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(54) Title: CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

(57) Abstract: The present invention provides three-dimensional structural information from the hyperthermophilic bacterium Aquifex aeolicus which is a histone deacetylase-like protein (HDLP). HDLP shares 35.2% amino acid sequence identity with human histone deacetylase (HDAC1). The present invention further provides three-dimensional structural information of HDLP bound by inhibitor molecules. The three-dimensional structural information of the present invention is useful to design, isolate and screen deacetylase inhibitor compounds capable of inhibiting HDLP, HDAC family members and HDLP-related molecules. The invention also relates to nucleic acids encoding a mutant HDLP which facilitates the determination of the three-dimensional structure of HDLP in the presence of a zinc atom.



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Crystal Structure of a Deacetylase and Inhibitors Thereof

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This application claims priority of U.S. Provisional Application No. 60/152,753, filed September 8, 1999, the contents of which are hereby incorporated by reference.

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This invention has been made with government support under National Institutes of Health Grant No. RO1 CA-65698. Accordingly, the U.S. Government may have certain rights in the invention.

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Throughout this application, various publications are referenced by author, date and citation. The disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art as known to those skilled therein as of the date of the invention described and claimed herein.

Introduction

25 The present invention relates to a histone deacetylase homologue from the hyperthermophilic bacterium Aquifex aeolicus, HDLP (histone deacetylase like protein; also known as AcuCl), which shares 35.2 % sequence identity with human histone deacetylase (HDACl), that can be co-crystallized with an inhibitory ligand, and more particularly, to the detailed crystallographic data obtained from said co-crystallization which is disclosed herein. The invention also relates to methods of using the crystal structure and x-ray crystallographic coordinates of the apo-HDLP and

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inhibitor-bound HDLP to design, isolate and screen compounds which bind to and inhibit the active site of HDLP and HDLPrelated proteins, such as those proteins belonging to the HDAC family, including HDAC1.

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Background of the Invention

The reversible modification of histones by acetylation is associated with changes in nucleosome conformation and chromatin structure, and plays an important role in the regulation of gene expression (reviewed in Davie and Chadee, 1998, J. Cell Biochem. Suppl. 30-31:203-213). The histone acetylase and deacetylase enzymes that carry out these modifications are involved in many cellular processes such as cell cycle progression and differentiation, and their deregulation is associated with several types of human cancer (reviewed in Kouzarides, 1999, Curr. Opin. Genet. Dev. 9:40-48; Hassig et al., 1997, Chem. Biol. 4:783-789; Fenrick and Heibert, 1998, J. Cell. Biochem. Suppl. 30-<u>31</u>:194-202).

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Recently, several experimental antitumor compounds, such as trichostatin A (TSA), trapoxin, suberoylanilide hydroxamic acid (SAHA), and phenylbutyrate have been shown to act, at least in part, by inhibiting histone deacetylases. Richon et al., 1998, Proc. Natl. Acad. Sci., USA 95:3003-3007; Yoshida 25 et al., 1990, J. Biol. Chem. <u>265</u>:17174-17179; Kijima et al., 1993, J. Biol. Chem. <u>268</u>:22429-22435. Additionally, diallyl sulfide and related molecules (Lea et al., 1999, $Int.\ J.$ Oncol. 2:347-352), oxamflatin (Kim et al., 1999, Oncogene 15:2461-2470), MS-27-275, a synthetic benzamide derivative (Saito et al., 1999, Proc. Natl. Acad. Sci. <u>96</u>:4592-4597),

butarate derivatives (Lea and Tulsyan, 1995, Anticancer Res. 15:879-883), FR901228 (Nokajima et al., 1998, Exp. Cell Res. 241:126-133), depudecin (Kwon et al., 1998, Proc. Natl. Acad. Sci. USA 95:3356-3361) and m-carboxysinnamic acid bishydroxamide (CBHA; Richon et al., Proc. Natl. Acad. Sci. USA 95:3003-3007) have been shown to inhibit histone deacetylases. In vitro, these compounds can inhibit the growth of fibroblast cells by causing cell cycle arrest in the G1 and G2 phases (Richon et al., 1996, Proc. Natl. Acad. USA 93:5705-5708; Kim et al., 1999, Oncogene 18:2461-2470; Yoshida et al., 1995, Bioessays 17:423-430; Yoshida & Beppu, 1988, Exp. Cell. Res. 177:122-131), and can lead to the terminal differentiation and loss transforming potential of a variety of transformed cell lines. Richon et al., 1996, Proc. Natl. Acad. Sci. USA 93:5705-5708; Kim et al., 1999, Oncogene 18:2461-2470; Yoshida et al., 1987, Cancer Res. 47:3688-3691. In vivo, phenylbutyrate is effective in the treatment of acute promyelocytic leukemia in conjunction with retinoic acid. Warrell et al., 1998, J. Natl. Cancer Inst. 90:1621-1625. SAHA is effective in preventing the formation of mammary tumors in rats, and lung tumors in mice. Desai et al., 1999, Proc. AACR 40: abstract #2396; Cohen et al., Cancer Res., submitted.

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Histone deacetylases catalyze the removal of acetyl groups from the ε -amino groups of lysine residues clustered near the N-terminus of nucleosomal histones, and this process is associated with transcriptional repression (reviewed in Struhl, 1998, Genes Dev. 12:599-606). Deletion of the yeast histone deacetylase gene, rpd3, or its pharmacological

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inactivation with trichostatin A reduces the transcriptional repression in a subset of promoters, such as those of Ume6-regulated genes. Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127. This is accompanied by the increased acetylation of H4 histones in the repressed promoter and its vicinity, but has no effect on histones at promoter distal regions. Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127; Rundlett et al., 1998, Nature 392:831-835.

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Histone deacetylases are recruited to specific promoters by associating with DNA-binding transcriptional repressors, either directly or through co-repressors that bridge the deacetylase to the transcriptional repressors. For example, the Mad and Ume6 repressors bind to the co-repressor Sin3A (Laherty et al., 1997, Cell 89:349-356; Hassig et al., 1997, Cell 89:341-347; Kadosh & Struhl, 1997, Cell 89:365-371), and the nuclear receptors bind N-CoR and the related SMRT co-repressors. Nagy et al., 1997, Cell 89:373-380; Alland et al, 1997, Nature 387:49-55; Heinzel et al, 1997, Nature 387:49-55; Heinzel et al, 1997, Nature

The deregulation of histone deacetylase recruitment appears to be one of the mechanisms through which these enzymes contribute to tumorigenesis. In acute promyelocytic leukemia (APL), chromosomal translocations fuse the retinoic acid receptor-α (RARα) to either PLZF or to PML. These fusion oncoproteins have aberrant transcriptional repression activity resulting, in part, through the recruitment of a co-repressor and, in turn, HDACs. Grignani et al, 1998, Nature 391:815-818; Lin et al., 1998, Nature 391:811-814. Treatment of PLZF-RARα APL cells with TSA enhances their

responsiveness to retinoic acid-induced differentiation. Grignani et al, 1998, Nature 391:815-818; Lin et al., 1998, Nature 391:811-814.

The histone deacetylases comprise a large family of 5 proteins, conserved from yeast to man, and are divided into two related classes. Class I is characterized by human HDAC1, 2, 3 (Taunton et al., 1996, Science 272:408-411; Yang et al., 1996, Proc. Natl. Acad. Sci. USA 93:12845-12850; Emiliani et al., 1998, Proc. Natl. Acad. Sci. USA 95:2795-10 2800), and yeast RPD3 (Videl & Gaber, 1991, Mol. Cell. Biol. 11:6317-6327), and class II by the human HDAC4, (Grozinger et al., 1999, Proc. Natl. Acad. Sci. USA 96:4868-4873; Fischle, et al., 1999, J. Biol. Chem. <u>274</u>:11713-11720), and yeast HDA1 (Rundlett et al., 1996, Proc. Natl. 15 The two classes share a Acad. Sci. USA <u>93</u>:14503-14508). ~390 amino acid region of sequence similarity, comprising the deacetylase core, but are divergent outside this region. The histone deacetylase genes belong to an even larger superfamily (Leipe & Landsman, 1997, Nucleic Acids Res. 20 the prokaryotic acetoin that contains 25:3693-3697) utilization proteins (AcuC; 28.1% sequence identity to HDAC1), and the prokaryotic acetylpolyamine amidohydrolases (APAH; 15.0 % sequence identity to HDAC1). The enzymatic activity of AcuC is not clear, but its disruption reduces 25 the ability of B. subtilis to breakdown acetoin and utilize it as a carbon source. Grundy et al., 1993, Mol. Microbiol. 10:259-271. APAHs catalyze the deacetylation of polyamines by cleaving a non-peptide amide bond (reviewed in Leipe & Landsman, 1997, Nucleic Acids Res. 25:3693-3697). 30

It is useful to address the questions of how HDACs and HDACrelated proteins catalyze the deacetylation of histones and how the above-referenced compounds, particularly those compounds with antitumor activity, inhibit this activity in order to better understand the mechanism of inhibition of HDACs and to facilitate discovery of additional useful compounds which may inhibit this activity. To this end, the present invention has determined the three dimensional structure of a HDAC1-like protein from the thermophilic bacterium Aquifex aeolicus, herein after HDLP. determination of the nucleic acid coding sequence of HDLP was described by Deckert et al., 1998, Nature 392:353-358. encoded 375 residue protein, whose sequence was The determined from the nucleic acid encoding sequence, shares 35.2% amino acid sequence identity with HDAC1, deacetylates histones in vitro, and is inhibited by TSA, SAHA and several other HDAC inhibitors. The determination of the threedimensional structure of HDLP is useful in the design, identification and screening of new HDAC family inhibitory compounds which are useful for the inhibition of cell growth both in vivo and in vitro.

Summary of the Invention

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In general, it is the object of the present invention to provide detailed three-dimensional structural information 25 for a family of proteins known as histone deacetylases (HDAC), and particularly a homoloque from the hyperthermophilic bacterium Aquifex aeolicus HDLP (histone deacetylase-like protein) which shares 35.2 % sequence identity with human histone deacetylase (HDAC1). It is also an object of the present invention to provide three-

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dimensional structural information of an HDLP bound to an inhibitory compound.

In one embodiment of the invention, three-dimensional structure information is obtained from a crystal of wildtype HDLP (SEQ ID NO:1) (the nucleic acid encoding wild-type HDLP is SEQ ID NO:2). In a further embodiment of the invention, three-dimensional information is obtained from a mutant HDLP comprising two mutations (1) cysteine 75 to a serine and (2) cysteine 77 to a serine (Cys75Ser/Cys77Ser double mutant; SEQ ID NO:3) (the nucleic acid encoding HDLP Cys75Ser/Cys77Ser double mutant is SEQ ID NO:4). The HDLP facilitates invention present of the mutant determination of three-dimensional structural information of HDLP bound to a zinc atom at its zinc atom-binding site.

In a preferred embodiment of the invention, the threedimensional structural information is obtained from a cocrystal of a protein-inhibitor compound complex that comprises HDLP or HDLP Cys75Ser/Cys77Ser double mutant and trichostatin A (TSA). In another preferred embodiment of the invention the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor HDLP HDLP orcomprises complex that compound suberoylanilide and mutant Cys75Ser/Cys77Ser double hydroxamic acid (SAHA). Any HDLP or HDLP-related protein (e.g. HDAC) inhibitor compound that may be co-crystallized with HDLP may be used to form a co-crystal of the present invention.

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The protein crystals and protein-inhibitory complex cocrystals of the present invention diffract to a high

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resolution limit of at least equal to or greater than 4 angstrom (Å). In a preferred embodiment, the protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high resolution limit of greater than 2.5 Å.

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A crystal of the present invention may take a variety of forms, all of which are contemplated by the present invention. In a preferred embodiment, the crystal has a space group of C2 with one molecule in the asymmetric unit and with unit dimensions of a = 51.4 Å, b = 93.8 Å, 78.7 Å and β = 96.9° (see, e.g., Example 2, below). another preferred embodiment, the crystal has a space group of $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of a=53.4 Å, b=94.4 Å, c=156.3 Å (see, e.g., Example 2, below). The HDLP structure comprises a parallel β sheet with α helices packing against both faces. At one end of the β sheet, the HDLP has a narrow, tube-like pocket formed by several well-ordered loops. The walls of the pocket are lined with hydrophobic residues and there is a zinc binding site and several polar side chains at the bottom of the pocket. The inhibitory compounds of the present invention bind in the pocket.

The three-dimensional structural information obtained from crystals of HDLP, HDLP Cys75Ser/Cys77Ser double mutant, HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom, HDLP comprising an inhibitory compound such as TSA or SAHA, and HDLP Cys75Ser/Cys77Ser double mutant comprising an inhibitor compound such as TSA or SAHA may be employed to solve the structure of any HDLP-related protein (e.g. HDAC) crystal,

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or any mutant HDLP-related protein and particularly any wild type or mutant of HDLP-related protein complexed with a ligand, including a substrate or inhibitor compound. If the crystals are in a different space group than the known structure, molecular replacement may be employed to solve the structure, or if the crystals are in the same space group, refinement and difference fourier methods may be employed. The structure of HDLP-related proteins (e.g. HDAC1) comprise no greater than a 2.0 Å root mean square deviation (rmsd) in the positions of the C α atoms for at least 50% or more of the amino acids of the full-length HDLP structure.

The present invention also provides a nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant having the amino acid sequence of SEQ ID NO:3 and the nucleic acid sequence of SEQ ID NO:4. It is also contemplated by the invention that mutations be made in HDLP-related proteins at cysteine residues, as with the Cys75Ser/Cys77Ser double mutant, in order to facilitate the determination of the structure of said proteins bound to a zinc atom. Additionally, the present invention provides expression vectors which comprise the nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant encoded by the sequence represented by SEQ ID NO:4 operatively linked to expression control sequences.

It is another object of the present invention to provide methods for the design, identification and screening of potential inhibitor compounds of the HDLP/HDAC family. In a preferred embodiment the method for the rational design,

identification and screening of potential inhibitor compounds for HDLP and HDLP-related proteins (e.g. HDACs) comprising deacetylase activity comprises the steps of: (a) using a three-dimensional structure of an HDLP as defined by the atomic coordinates of the present invention; employing said three-dimensional structure to design or select said potential inhibitor compound; (c) synthesizing and/or selecting said potential inhibitor; (d) contacting said potential inhibitor compound with said enzyme in the presence of acetylated substrate; and (e) determining the percent inhibition of deacetylase activity to determine the inhibitory activity of said potential inhibitor compound. In a further preferred embodiment, the binding properties of said rationally designed inhibitory compound may be determined by a method comprising the steps of: (a) forming a complex comprising said inhibitory compound and HDLP or a HDLP-related protein, (b) co-crystallizing said inhibitory compound-HDLP complex; (c) determining said dimensional structure of said co-crystal through molecular replacement or refinement and difference fourier with the molecular coordinates of HDLP as defined by the present invention; and (d) analyzing the three-dimensional structure to determine the binding characteristics of said potential inhibitor compound.

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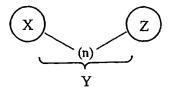
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It is a further object of the present invention to identify a defined class of HDLP/HDAC family inhibitor compounds. The HDLP/HDAC family inhibitor compounds of the present invention are represented by formula (I):

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(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises and active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and may further bind to a zinc atom.

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Brief Description of the Drawings

Figure 1 is a table listing the statistics from the X-ray crystallographic analysis of a HDLP crystal, a HDLP-TSA co-crystal, and a HDLP-SAHA co-crystal.

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Figure 2 shows an alignment of various HDAC homologues with percent sequence identity depicted.

Figure 3 shows a graph indicating the histone deacetylase activity of HDLP and HDAC1 and the inhibition of HDLP and HDAC1 by the inhibitors TSA and HC-toxin.

Figure 4 shows (A & B) a schematic representation of the HDLP-Zn²⁺-TSA complex in two approximately orthogonal views,

(C) a topology diagram of HDLP indicating the regions of homology with HDAC1, and (D) a close-up schematic representation of the HDLP-Zn²⁺-SAHA complex.

Figure 5 shows (A) a schematic representation of a slice through a surface representation of HDLP with the pocket internal cavities and position of the β sheet indicated, (B) a schematic representation of a close-up view of the active site looking down into the pocket in an orientation similar to Figure 4B.

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Figure 6 shows (A) a space-filling representation of TSA in the active site pocket, (B) a closeup stereo view of the structure of the $HDLP-ZN^{2+}-TSA$ complex in a similar orientation to Figure 4B, and (C) a schematic representation of the HDLP-TSA interactions.

Figure 7 shows (A) a schematic representation of the regions of homology shared between HDLP and HDAC1 in an orientation similar to that of Figure 4A, and (B) a detailed schematic representation of the homology shared in the pocket and internal cavity between HDLP and HDAC1 in an orientation similar to that of Figure 4B.

Figure 8 shows a schematic representation of the proposed catalytic mechanism for the deacetylation of acetylated lysine.

Figure 9 shows a schematic representation of a space filling diagram showing the conserved amino acids in the active site and nearby grooves.

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Figure 10 is the nucleic acid sequence of HDLP from Aquifex aeolicus (SEQ ID NO. 2).

Figure 11 is the amino acid sequence of full length HDLP from Aquifex aeolicus (SEQ ID NO. 1).

Figure 12 is the nucleic acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 6).

Figure 13 is the amino acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 5).

Figure 14 is the nucleic acid sequence of a double mutant of HDLP from Aquifex aeolicus comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 4).

Figure 15 is the amino acid sequence of a double mutant of HDLP from Aquifex aeolicus comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 3).

Figure 16-1 to 16-49 lists the atomic structure coordinates for HDLP as derived by X-ray diffraction from a crystal of HDLP.

Figure 17-1 to 17-49 lists the atomic structure coordinates

for HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc
atom in the active site as derived by X-ray diffraction from
a crystal of the HDLP Cys75Ser/Cys77Ser double mutant.

Figure 18-1 to 18-99 lists the atomic structure coordinates

for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray
diffraction from a co-crystal of HDLP complexed with TSA.

Figure 19-1 to 19-48 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with SAHA.

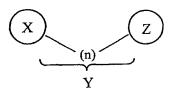
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Detailed Description of the Invention

The present invention provides crystals of a histone deacetylase (HDAC) homologue grown in the presence and absence of a compound capable of inhibiting the histone deacetylase activity of said HDAC homologue. As referred to herein, a HDAC homologue (as well as a HDLP-related protein) is any protein molecule having (a) greater than 15% sequence identity to over the 375 amino acid residues of HDLP; (b) having no more than twenty insertions or deletions for a total of no more than 100 amino acids; and (c) deacetylase activity. Sequence identity is calculated by the program DNAstar™ using the identity matrix weighing scheme clustal method (DNAstar program, Madison, WI).

A HDLP/HDAC inhibitor compound, as used herein, refers to any compound represented by Formula (I):

(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of tyrosine, proline and leucine; Y comprises an aliphatic chain group from about 5 to about 10 Å, preferably 7 Å, which binds to at least one amino acid selected from the group consisting of phenylalanine and glycine; and Z comprises a active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and which may further bind to a zinc atom. The HDAC inhibitory compounds of the present

invention can inhibit greater than 50% of the histone deacetylase activity of a HDAC homologue or a HDLP-related protein.

To grow the crystals of the present invention, the HDAC and HDAC-inhibitory compound complex are purified to greater than 80% total protein and more preferably purified to greater than 90% total protein. For expression and purification purposes, the full-length HDLP (Genbank accession number AE000719) may be subcloned from Aquifex aeolicus chromosomal DNA preparation by the polymerase chain reaction (PCR) and inserted into an expression vector.

A large number of vector-host systems known in the art may be used. Possible vectors include, but are not limited to, 15 plasmids or modified viruses, but the vector system must be compatible with the host cell used. Examples of vectors include E. coli bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid 20 derivatives, e.g., pGEX vectors (Amersham-Pharmacia, Piscataway, New Jersey), pET vectors (Novagen, Madison, WI), pmal-c vectors (Amersham-Pharmacia, Piscataway, New Jersey), pFLAG vectors (Chiang and Roeder, 1993, Pept. Res. 6:62-64), baculovirus vectors (Invitrogen, Carlsbad, CA; Pharmingen, 25 San Diego, CA), etc. The insertion into a cloning vector can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini, by blunt end ligation if no complementary cohesive termini are available or by through nucleotide linkers using techniques standard in the art. 30 Ausubel et al. (eds.), Current Protocols in Molecular

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Biology, (1992). Recombinant vectors comprising the nucleic acid of interest may then be introduced into a host cell compatible with the vector (e.g. E. coli, insect cells, mammalian cells, etc.) via transformation, transfection, infection, electroporation, etc. The nucleic acid may also be placed in a shuttle vector which may be cloned and propagated to large quantities in bacteria and then introduced into a eukaryotic cell host for expression. The vector systems of the present invention may provide expression control sequences and may allow for the expression of proteins in vitro.

In a preferred embodiment, the full length HDLP (SEQ ID NO:2) is subcloned from Aquifex aeolicus chromosomal DNA preparation into pGEX4T3 (Amersham-Pharmacia, Piscataway, New Jersey). In order to construct a double mutant comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO:4), and to construct the HDLP active site mutant Tyr297Phe (SEQ ID NO:5 and SEQ ID NO:6), PCR site directed mutagenesis may be employed with verification by DNA sequencing by methods known to those skilled in the art (see, e.g., Example 1 below). The mutants of the present invention may be subcloned into a suitable expression vector and introduced into a host cell for protein production, as described above.

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The HDLP nucleic acids of the present invention may be subcloned into an expression vector to create an expression construct such that the resultant HDLP molecule which is produced comprises a fusion protein wherein said fusion protein comprises a tag for ease of purification. As referred to herein, a "tag" is any additional amino acids

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which are provided in a protein either c-terminally, nterminally or internally for the ease of purification, for the improvement of production or for any other purpose which may facilitate the goals of the present invention (e.g. to achieve higher levels of production and/or purification). Such tags include tags known to those skilled in the art to be useful in purification such as, but not limited to, his tag, glutathione-s-transferase tag, flag tag, mbp (maltose binding protein) tag, etc. In a preferred embodiment, the wild-type and mutant HDLPs of the present invention are tagged with glutathione-s-transferase (see Example 1 below). In another preferred embodiment, HDAC1 is flag tagged (see Example 1 below). Such tagged proteins may also be engineered to comprise a cleavage site, such as a thrombin, enterokinase or factor X cleavage site, for ease of removal of the tag before, during or after purification. systems which provide a tag and a cleavage site for removal of the tag are particularly useful to make the expression constructs of the present invention.

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The tagged HDLPs and HDACs of the present invention may be purified by immuno-affinity or conventional chromatography, including but not limited to, chromatography employing the following: glutathione-sepharose™ (Amersham-Pharmacia. Piscataway, New Jersey) or an equivalent resin, nickel or cobalt-purification resins, anion exchange chromatography, cation exchange chromatography, hydrophobic resins, gel filtration, antiflag epitope resin, reverse chromatography, etc. After purification, the HDLP and HDLPinhibitor compound complex may be concentrated to greater than 1 mg/ml for crystallization purposes. In a preferred embodiment HDLP and HDLP-inhibitor complexes are

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concentrated to greater than 10 mg/ml for crystallization and in a particularly preferred embodiment, HDLP and HDLP-inhibitor complexes are concentrated to greater than 20 mg/ml.

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In order to determine whether the purified HDLPs of the present invention demonstrate histone deacetylase activity, the purified HDLPs and also any HDLP-related protein may be assayed by any method known to those skilled in the art for In a preferred the determination of said activity. embodiment, the purified HDLPs of the present invention are incubated in the presence of [3H]acetyl-labeled histone substrate (Carmen et al., 1996, J. Biol. Chem. 271:15837-15844) in a buffer suitable for detection of histone deacetylase activity (see Example 3 below); stopping the reaction; extracting the released acetate and measuring said released acetate, as described by Henzel et al. (J. Biol. Chem. 266:21936-21942 (1991); Example 3 below). preferred embodiment, the HDLPs of the present invention are inclubated in the presence of ZnCl2 in order to obtain histone deacetylase activity therefrom (Example 3 below).

In another embodiment, the crystals of the present invention comprise purified wild-type HDLP (SEQ ID NO:1) and are grown at room temperature by the hanging-drop vapor-diffusion method from a crystallization solution comprising one or more precipitants selected from the group consisting of isopropanol, polyethylene glycol, and tert butanol (see Example 2 below). The crystallization solution may further comprise one or more salts including salts selected from the group consisting of NaCl and KCl, and one or more buffers

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including buffers selected from the group consisting of Tris (tris(hydroxymethyl)aminomethane and bis-tris propane-Cl (1,3-bis[tris(hydroxymethyl)methyl-amino] propane) (see Example 2 below). The pH of the crystallization solution is preferably between pH 5 to 9, although other pH values are also contemplated by the present invention (see Example 2 below).

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Any crystallization technique known to those skilled in the art may be employed to obtain the crystals of the present invention, including, but not limited to, batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and micro dialysis. Seeding of the crystals in some instances may be required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used.

The crystals of the present invention may form in the space group C2 with one molecule in the asymmetric unit and with unit dimensions of a=51.4 Å, b=93.8 Å, c=78.7 Å and $\beta=96.9^{\circ}$ (see Example 2 below). The crystals of the present invention may also form in the space group $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of a=53.4 Å, b=94.4 Å, c=156.3 Å (see Example 2 below). However, the present invention contemplates crystals which form in any space group including, but not limited to, C2, $P2_1$, $P2_12_12_1$, $P3_121$, $P4_32_12_1$, and $C222_1$. The crystals diffract to a resolution greater than 4 Å, preferably greater than 2.5 Å.

To collect diffraction data from the crystals of the present

invention, the crystals may be flash-frozen in the crystallization buffer employed for the growth of said crystals, however with preferably higher precipitant concentration (see, e.g., Example 2 below). For example, but not by way of limitation, if the precipitant used was 28% PEG 1500, the crystals may be flash frozen in the same crystallization solution employed for said crystal growth wherein the concentration of the precipitant is increased to 35% (see Example 2 below). If the precipitant is not a sufficient cryoprotectant (i.e. a glass is not formed upon cryoprotectants (e.g. glycerol, flash-freezing), molecular weight PEGs, alcohols, etc) may be added to the solution in order to achieve glass formation upon flashfreezing, providing the cryoprotectant is compatible with preserving the integrity of the crystals. The flash-frozen crystals are maintained at a temperature of less than -110°C and preferably less than -150°C during the collection of the crystallographic data by X-ray diffraction. diffraction data may be processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, Method Ensemble. 276:307-326) but any method known to those skilled in the art may be used to process the X-ray diffraction data.

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In order to determine the atomic structure of HDLP according to the present invention, multiple isomorphous replacement (MIR) analysis, model building and refinement may be performed. For MIR analysis, the crystals may be soaked in heavy-atoms to produce heavy atom derivatives necessary for MIR analysis. As used herein, heavy atom derivative or derivitization refers to the method of producing a chemically modified form of a protein or protein complex

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crystal wherein said protein is specifically bound to a heavy atom within the crystal. In practice a crystal is soaked in a solution containing heavy metal atoms or salts, or organometallic compounds, e.g., lead chloride, gold cyanide, thimerosal, lead acetate, uranyl acetate, mercury chloride, gold chloride, etc, which can diffuse through the crystal and bind specifically to the protein. location(s) of the bound heavy metal atom(s) or salts can be determined by X-ray diffraction analysis of the soaked This information is used to generate MIR phase crystal. information which is used to construct the three-dimensional structure of the crystallized HDLPs and HDLP-related proteins of the present invention. In a preferred embodiment, the heavy atoms comprise thimerosal, $KAu(CN)_2$ and $Pb (Me)_3 OAc$ (see Example 2 below). The MIR phases may be calculated by any program known to those skilled in the art and preferably with the program MLPHARE (The CCP4 suite: Programs for computational crystallography, 1994, Crystallogr. D. 50:760-763) and may also use the anomalous diffraction signal from the thimerosal derivative. preferred embodiment, the MIR phases were calculated at 2.5 Å and have a mean figure of merit of 0.55 (see Figure 19 and Example 2 below). The phases may be improved where necessary by solvent flattening by methods known to those skilled in the art including, but not limited to, through the use of the program DM (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D <u>50</u>:760-763).

Thereafter, an initial model of the three-dimensional structure may be built using the program O (Jones et al.,

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1991, Acta Crystallogr. A 47:110-119). The interpretation and building of the structure may be further facilitated by use of the program CNS (Brunger et al., 1998, Acta Crystallogr. D 54:905-921).

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For the determination of the HDLP-inhibitor compound complex structure, if the space group of the HDLP-inhibitor compound complex crystal is different, molecular replacement may be employed using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure whose structure may be determined as described above and below in Example 2. the space group of the HDLP-inhibitor compound crystals is the same, then rigid body refinement and difference fourier may be employed to solve the structure using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure.

The term "molecular replacement" refers to a method that involves generating a preliminary model of the three-dimensional structure of the HDLP crystals of the present invention whose structure coordinates are unknown prior to the employment of molecular replacement. Molecular replacement is achieved by orienting and positioning a molecule whose structure coordinates are known (in this case the previously determined apo-HDLP) within the unit cell as defined by the X-ray diffraction pattern obtained from an HDLP or HDLP-related protein crystal whose structure is

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unknown so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of several forms of refinement to provide a final, accurate structure.

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Any method known to the skilled artisan may be employed to determine the structure by molecular replacement. example, the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D. 50:760-763) may be employed to determine the structure of an unknown histone deacetylase +/- an inhibitor by molecular replacement using the apo-HDLP coordinates (Figure 16). For the structure determination of the inhibitory compound TSA, the structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST, http://www.ccdc.cam.ac.uk >>) may be employed to define the stereochemical restraints used in the refinement with the program CNS (Brunger et al., 1998, Acta Crystallogr. D <u>54</u>:905-921).

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP are useful for solving the structure of crystallized proteins which belong to the HDAC family by molecular replacement. Similarly, any structure of a crystallized protein which is thought to be similar in structure based on function or sequence similarity or identity to HDLP may be solved by molecular replacement with the HDLP structural

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The structure of information of the present invention. HDLP-related proteins as determined by molecular replacement as described above and in Example 2 below, comprise a root mean square deviation (rmsd) of no greater than 2.0 $\hbox{\normale A}$ in the positions of $C\alpha$ atoms for at least 50% or more of the amino acids of the structure over the 375 residues of full-length HDLP. Such a rmsd may be expected based on the amino acid sequence identity. Chothia & Lesk, 1986, Embo J. 5:823-826.

The refined three-dimensional HDLP structures of the present invention, specifically apo-HDLP, Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site, HDLP/TSA complex comprising a zinc atom in the active site, and HDLP/SAHA complex comprising a zinc atom in the active site, are represented by the atomic coordinates set forth in Figures 16 to 19 respectively. The refined model for apo-HDLP comprising amino acids 1-375 consists of wild-type HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution model refined Similarly, the Å. 1.8 Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site also consists of residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 2.0 Å. The refined model for the HDLP/TSA complex comprising a zinc atom in the active site consists of the Cys75Ser/Cys77Ser double mutant HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered, has TSA in the binding pocket and was determined to a resolution of 2.1 Å. HDLP/SAHA complex is similar to the HDLP/TSA complex but has 30 SAHA in the binding pocket and was determined to a resolution of 2.5 Å.

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For the purposes of further describing the structure of HDLP and HDLP-related proteins, including, but not limited to, HDACs, from the data obtained from the HDLP crystals of the present invention, the definition of the following terms is provided:

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The term " β sheet" refers to two or more polypeptide chains (or β strands) that run alongside each other and are linked in a regular manner by hydrogen bonds between the main chain C=O and N-H groups. Therefore all hydrogen bonds in a beta-sheet are between different segments of polypeptide. Most β -sheets in proteins are all-parallel (protein interiors) or all-antiparallel (one side facing solvent, the other facing the hydrophobic core). Hydrogen bonds in antiparallel sheets are perpendicular to the chain direction and spaced evenly as pairs between strands. Hydrogen bonds in parallel sheets are slanted with respect to the chain direction and spaced evenly between strands.

The term " α helix" refers to the most abundant helical 20 conformation found in globular proteins. The average length of an α helix is 10 residues. In an α helix, all amide protons point toward the N-terminus and all carbonyl oxygens point toward the C-terminus. The repeating nature of the phi, psi pairs ensure this orientation. Hydrogen bonds 25 within an $\boldsymbol{\alpha}$ helix also display a repeating pattern in which the backbone C=O of residue X (wherein X refers to any amino acid) hydrogen bonds to the backbone HN of residue X+4. The α helix is a coiled structure characterized by 3.6 residues per turn, and translating along its axis 1.5 Å per 30 amino acid. Thus the pitch is 3.6x1.5 or 5.4 Å. The screw sense of alpha helices is always right-handed.

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The term "loop" refers to any other conformation of amino acids (i.e. not a helix, strand or sheet). Additionally, a loop may contain bond interactions between amino acid side chains, but not in a repetitive, regular fashion.

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Amino acid residues in peptides shall herein after be abbreviated as follows: Phenylalanine is Phe or F; Leucine is Leu or L; Isoleucine is Ile or I; Methionine is Met or M; Valine is Val or V; Serine is Ser or S; Proline is Pro or P; Threonine is Thr or T; Alanine is Ala or A; Tyrosine is Tyr or Y; Histidine is His or H; Glutamine is Gln or Q; Asparagine is Asn or N; Lysine is Lys or K; Aspartic Acid is Asp or D; Glutamic Acid is Glu or E; Cysteine is Cys or C; Tryptophan is Trp or W; Arginine is Arg or R; and Glycine is Gly or G. For further description of amino acids, please refer to Proteins: Structure and Molecular Properties by Creighton, T.E., W.H. Freeman & Co., New York 1983.

The term "positively charged amino acid" refers to any amino

physiological conditions. Examples of positively charged amino acids are Arg, Lys and His. The term "negatively charged amino acid" refers to any amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged amino acids are Asp and Glu. The term "hydrophobic amino acid" refers to any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of hydrophobic amino acids are Ala, Leu, Ile, Gly, Val, Pro, Phe, Trp and Met. The term "hydrophilic amino acid" refers to any amino acid having an uncharged, polar side chain that is

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relatively soluble in water. Examples of hydrophilic amino acids are Ser, Thr, Tyr, Asp, Gln, and Cys. The term "aromatic amino acid" refers to any amino acid comprising a ring structure. Examples of aromatic amino acids are His, Phe, Trp and Tyr.

The term "charge relay system" refers to a His-Asp arrangement as described by Fersht & Sperling, 1973, J. Mol. Biol. 74:137-149; Blow et al., 1969, Nature 221:337-340.

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information The obtained from the three-dimensional structures of the present invention reveal that HDLP has a single-domain structure that belongs to the open α/β class of folds (see, e.g., Branden, 1980, Q. Rev. Biophys. 13:317-38). Two orthogonal views of the overall three-15 dimensional structure of HDLP are depicted in Figure 4A and The HDLP structure has a central eight-stranded 4B. parallel β sheet (strands arranged as $\beta 2 - \beta 1 - \beta 3 - \beta 8 - \beta 7 - \beta 4 - \beta 5$ and sixteen lpha helices (labeled lpha1 through lpha16 respectively). See Figure 4C. Four of the helices pack on 20 either face of the β sheet (α 7, α 8, α 9, α 10 and α 11, α 12, $\alpha 13\,,~\alpha 14)$ forming the core $~\alpha/\beta$ structure characteristic of this class of folds. Most of the remaining eight helices are positioned near one side of the β sheet, near stands $\beta2\text{--}$ β 1- β 3- β 8. Large, well defined loops (Loops L1-L7; Figure 25 4C) originate from the C-terminal ends of the β -strands. The extra helices and the large L1-L7 loops are associated with a significant extension of the structure beyond the core α/β motif. This extension of the structure gives rise to two prominent architectural features: a deep, narrow 30 pocket and an internal cavity adjacent to the pocket. These

two architectural features comprise the active site (see Figure 5A). The structure of HDLP-related proteins (e.g. HDACs) may also comprise the conserved α/β structure characteristic.

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The term "active site" comprises any or all of the following sites in HDLP, the substrate binding site, the site where the cleavage of an acetyl group from a substrate occurs or the site where an inhibitor of the HDAC family or, more particularly, HDLP binds. The active site, as referred to herein, comprises Aspl66, Asp258, His170, Tyr297, His131, His132, Asp168, Asp173, Phe141, Phe198, Leu265, Pro22 and Gly140, and also a metal bound at the bottom of the pocket by Asp173, Asp168 and His defined by the coordinates listed in Figures 16 to 19 with an rmsd of 2.0 Å. The metal which binds at the bottom of the pocket will be a divalent cation selected from the group consisting of zinc, cobalt or manganese.

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The deep narrow pocket has a tube-like shape with a depth of ~ 11 Å. The pocket opening constricts half way down to ~ 4.5 by 5.5 Å, and becomes wider at the bottom (see Figure 5A). The pocket and its immediate surroundings are made up of loops L1 through L7.

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The walls of the pocket are covered with side chains of hydrophobic and aromatic residues (Pro22, Tyr91 near the entrance; and Gly140, Phe141, Phe 198, Leu265 and Tyr297 further down; Figure 5B). For numbering of amino acids please refer to SEQ ID NO:1. Of particular interest are Phe141 and Phe198, whose phenyl groups face each other in

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parallel at a distance of 7.5 Å, marking the most slender portion of the pocket (see Figure 5B). Of particular interest is that only one pocket residue differs in HDAC1 when the sequences are aligned (alignment may be accomplished using DNAstar™ MegAlign™ program, Madison, WI), this residue is Glu98 of HDAC1 which is Tyr91 in HDLP. The structure reveals that this residue in HDLP is mostly solvent exposed.

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Near the bottom of the pocket of the active site at its narrowest point, is located a zinc ion (see Figure 6A). In order to obtain the zinc in the structure, the crystals may be soaked in zinc (e.g. ZnCl₂) or co-crystalized in the presence of zinc. The zinc ion is coordinated by Aspl68 (Oδ1, 2.1 Å), His170 (Nδ1, 2.1 Å), Asp258 (Oδ1, 1.9 Å) and a water molecule (2.5 Å). See Figure 5B and 6B. The amino acid residues that coordinate zinc are arranged in a tetrahedral geometry, but the position of the water molecule, which is also hydrogen bonded to His131, deviates from this geometry by -25°.

In addition to the zinc ligands, the bottom of the pocket contains two histidine (His131 and His132), two aspartic acids (Asp166 and Asp173) and a tyrosine (Tyr297). See Figure 5B and 10B. Each of the histidines makes a hydrogen bond through its Nol to an aspartic acid carboxylate oxygen, with the oxygen located in the plane of the imidizole ring (Figure 5B). This His-Asp arrangement is characteristic of the charge relay system present in the active sites of serine proteases, where it serves to polarize the imidizole Ne and increase its basicity. Fersht & Sperling, 1973, J.

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Mol. Biol. <u>74</u>:137-149; Blow et al., 1969, Nature <u>221</u>:337-340.

The Asp166-His131 charge pair relay (hereafter referred to as "buried charged relay") is positioned even deeper in the pocket and more buried compared to the Asp173-His132 charge relay (hereafter referred to as "exposed charge relay") which is partially solvent exposed. The buried charge relay makes a hydrogen bond (2.6 Å) to the zinc-bound water molecule referred to above, and this hydrogen bond could contribute to the deviation of the water-zinc coordination from ideal geometry (Figure 5B). The exposed charge relay is directed to a point ~ 2.5 Å away from the water molecule and closer to the surface.

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Tyr 297 is positioned next to the zinc, opposite from where the two charge relay systems are located. The Tyr hydroxyl group lies 4.4 Å away from the zinc atom and has no interactions with the rest of the protein (Figure 5B). Next to Tyr297, there is an opening in the pocket wall, which leads to the adjacent internal cavity.

The floor of the internal cavity is made up of portions of the L3 and L7 loops as they emerge from the β strands, and the roof is made up by the $\alpha 1\text{-L} 1\text{-}\alpha 2$ segment. The L1 loop appears more flexible than other loops in the structure. This may allow the transient exchange of the cavity contents with the bulk solvent.

The cavity is lined primarily with hydrophobic residues and is particularly rich in glycine residues (Ala127, Gly128, Gly129, Met130, and Phe141 of L3; Gly293, Gly294, Gly295 and

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Gly296 of L7; and Tyr17, Pro22 and Leu23 of L1). There are only two charged residues in the cavity (Arg27 and His 21) and these are contributed by the L1 loop.

The cavity may provide space for the diffusion of the acetate product away from the catalytic center, which may otherwise be crowded and shielded during deacetylation from the solvent when the substrate is bound. Such a role for the cavity is supported by the observation that the cavity contains three water and two isopropanol molecules (from the crystallization buffer) in the 1.8 Å apo-protein structure. The cavity may also bind another cofactor, in addition to zinc, for the facilitation of the enzymatic activity of the HDLP. A proposed catalytic mechanism for deacetylation is provided in Figure 8.

The structure of HDLP as defined by the present invention, in conjunction with the HDAC1 sequence homology, shows that the 375-amino acid HDLP protein corresponds to the histone deacetylase catalytic core which is conserved across the HDAC family (see Figure 2). The 35.2% HDLP-HDAC1 sequence identity predicts structural similarity with a rmsd in $\ensuremath{\text{C}\alpha}$ positions of ~ 1.5 Å. Chothia and Lesk describe the relation between the divergence of sequence and structure of proteins in Embo J. $\underline{5}$:823-826 (1986). residue C-terminus of HDLP is likely to have a divergent structure since this region has lower homology to HDAC1, although the $\alpha 16$ helix in this region is part of the conserved open α/β core fold and HDAC1 is likely to comprise a similar helix. However divergent this C-terminal region may be, this region is outside the active site and is likely to not effect the structure of the active site. Beyond the

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C-terminus of the histone deacetylase catalytic core, HDAC family members are divergent in length and sequence. In the HDAC family, this region (amino acid residues -390-482) is highly polar, populated with acidic residues, and is likely to be flexible or loosely folded.

The HDLP-HDAC homology maps primarily to the hydrophobic core and to the L1-L7 loops, with portions of the loops that make up the pocket and adjacent cavity having the highest level of amino acid residue sequence conservation (Figure 9A Specifically, all of the polar residues in the and 9B). active site (the zinc ligands, the two charge relay systems, and Tyr297) and the hydrophobic residues that make up the walls of the pocket (Gly140, Phe141, Phe198 and Leu265) are Among the residues that make up the internal identical. cavity, the ones closest to the active site are either identical or conservatively substituted (for example, Leu23 ightarrow Met and Met130ightarrow Leu). Surface residues around the pocket are conserved to a lesser extent, but are still above 35% average sequence identity.

The information obtained from the inhibitor-bound HDLP complex crystal structures of the present invention reveal detailed information which is useful in the design, isolation, screening and determination of potential inhibitor compounds which may inhibit HDLP/HDAC family members. As described above, the HDLP structure consists of a parallel β sheet with α helices packing against both faces (Figure 4A, 4B, and 4C). At one end of the β sheet, 7 loops (L1-L7) form a narrow, tube-like pocket which are lined with hydrophobic residues and which comprise a zinc binding site, several polar side chains, including two Asp-His charge

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relay systems. Mutation of the zinc ligands and other polar residues at the pocket bottom reduces or eliminates the catalytic activity.

The present inventors found that mutation at the Tyr297Phe site reduced activity. See also, Hassig et al., 1998, Proc. Natl. Acad. Sci. USA 95:3519-3524; Kadosh & Struhl, 1998, Genes Dev. 12:797-805. The elimination of activity by mutation of these residues indicates that this region is the enzyme active site. Adjacent to the active site, there is an internal cavity that may provide space for the diffusion of the acetate reaction product. Homology at the active site between HDLP and HDAC1, as described above, indicates that they share structural and functional homology.

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The inhibitor compound, trichostatin A (TSA) (Tsuji et al., 1976, J. Antibiotics 29:1-6) binds HDLP by inserting its long aliphatic chain, which has a hydroxamic acid group at one end, into the pocket (Figure 6A, 6B and 6C). aliphatic chain makes multiple contacts in the well-like, hydrophobic portion of the pocket. The hydroxamic acid reaches the polar bottom of the pocket, where it coordinates the zinc in a bidentate fashion and also forms hydrogen bonds with the polar residues in the active site, including the two charge relay system histidines. The aromatic dimethylamino-phenyl group at the other end of the TSA chain makes contacts at the pocket entrance and serves to cap it. The amino acid residues of HDLP which contact TSA are conserved in HDAC, indicating that TSA binds and inhibits HDAC in a similar fashion to HDLP.

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In the complex, the hydroxamic acid, most of the aliphatic chain and part of the dimethylamino-phenyl group of TSA are buried (60% of TSA's surface area; Figure 6A). The hydroxamic acid group binds the zinc in a bidentite fashion forming bonds through its carbonyl (2.4 Å) and hydroxyl groups (2.2 Å) resulting in a penta-coordinated Zn²+ (Figure 6B and 6C). The hydroxamic acid hydroxyl group replaces the water molecule that binds to the zinc in the apo-HDLP structure described above. The hydroxamic acid also hydrogen bonds with both charge relay system histidines (hydroxyl oxygen to His131 Ne2, 2.8 Å; and nitrogen to His132 Ne2, 2.8 Å), and the Tyr297 hydroxyl group (2.4 Å; Figure 6B and 6C).

The 5-carbon long branched alkene chain of TSA fits snugly in the narrow portion of the pocket making multiple van der Waals contacts with all of the hydrophobic groups lining the pocket (Figure 6B and 6C). Near its center, the chain contains a methyl substituted carbon-carbon double bond which is sandwiched between the phenyl groups of the Phel41 and Phe98 at the tightest point of the pocket (Figure 6A and 6B). The length of the alkene chain appears optimal for spanning the length of the pocket, and allowing contacts both at the bottom and at the entrance of the pocket, although, the cap group of Formula (I) may provide length to span the pocket allowing for a shorter alkene chain (aliphatic chain).

At the entrance of the pocket, one face of the planar structure formed by the dimethylamino-phenyl and adjacent carbonyl groups of TSA makes contacts at the rim of the pocket (Pro22, Tyr91, Phe141; Figure 6B and 6C). This

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packing is facilitated by the roughly 110° angle in the overall structure of TSA at the junction of the aliphatic chain and the dimethylamino-phenyl group (occurring at the sp³ hybridized C8 carbon). Upon TSA binding, the side chain of Tyr91, which is mostly solvent exposed, changes conformation to make space for the dimethylamino-phenyl group. This is the only change near the active site observed upon TSA binding.

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The hydroxamic acid group is a common motif in zinc 10 metalloprotease inhibitors. See U.S. Patent No. 5,919,940 and 5,917,090; See also, Grams et al., 1995, Biochemistry 34:14012-14020; Lovejoy et al., 1999, Nat. Struct. Biol. 6:217-221; and Holmes & Matthews, 1981, Biochemistry 20:6912-6920. Like TSA, these inhibitors also coordinate 15 the active site zinc in a bidentate fashion using their hydroxamate hyroxyl and carbonyl oxygens, replace the nucleophilic water molecule with their hydroxamate hydroxyl groups and form hydrogen bonds to the general base (Grams et al., 1995, Biochemistry 34:14012-14020; Lovejoy et al., 20 1999, Nat. Struct. Biol. 6:217-221; and Holmes & Matthews, 1981, Biochemistry 20:6912-6920).

SAHA, which has a ~30-fold weaker inhibitory activity than

TSA (Richon et al., 1998, Proc. Natl. Acad. Sci. USA

95:3003-3007), binds HDLP similarly to TSA (see, e.g.,

Figure 4D). The SAHA hydroxamic acid group makes the same

contacts to the zinc and active site residues, and the

importance of these interactions is underscored by the loss

of activity of SAHA derivatives lacking the hydroxamic group

(Richon et al., 1998, Proc. Natl. Acad. Sci. USA 95:3003-

the tube-like hydrophobic portion of the pocket. Compared to TSA however, SAHA's aliphatic chain packs less snugly and makes fewer van der waals contacts, in part, because SAHA lacks TSA's C15 methyl group branch. SAHA also lacks TSA's double bonds in this region, and this may lead to increased flexibility of the aliphatic chain. The cap group of SAHA consists of a phenyl-amino ketone group. In the crystal structure, the phenyl group has weak electron density, suggesting that it does not pack as well as the cap group of TSA. This may be due to the larger separation between the hydroxamic and cap groups of SAHA compared to TSA (compare TSA, Formula (II) and SAHA, Formula (III), below).

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25 (III)

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The determination of the structure of HDLP and HDLP bound to an inhibitory compound has enabled, for the first time, the identification of the active site of HDLP and of related HDLP proteins, such as proteins belonging to the HDAC family.

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP bound to an inhibitory compound is useful in rational drug design providing for a method of identifying inhibitory compounds which bind to and inhibit the enzymatic activity of HDLP, HDAC family proteins and other histone deacetylaselike proteins related to HDLP. Said method for identifying potential inhibitor for an enzyme comprising deacetylase activity comprises the steps of (a) using a three-dimensional structure of HDLP as defined by its atomic coordinates listed in Figure 16 to 19; (b) employing said three-dimensional structure to design or select said potential inhibitor; (c) synthesizing said potential inhibitor; (d) contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and (e) determining the ability of said inhibitor to inhibit said deacetylase activity.

The potential HDLP and HDLP-related (e.g. HDAC) inhibitors identified by the method of the present invention are represented by formula (I)

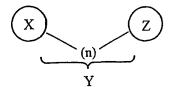
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(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and wherein Z may further bind to a zinc atom and with the provision that the compound of Formula (I) is not TSA, trapoxin, SAHA, SAHA derivatives described in U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5840,960 and 5,668,179.

The present invention permits the use of molecular design 20 techniques to design, identify and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site of HDLP and HDLPrelated proteins. The atomic coordinates of apo-HDLP and inhibitor-bound HDLP may be used in conjunction with 25 computer modeling using a docking program such as GRAM, DOCK, HOOK or AUTODOCK (Dunbrack et al., 1997, Folding & Design 2:27-42) to identify potential inhibitors of HDLP and This procedure can HDLP-related proteins (e.g. HDAC1). include computer fitting of potential inhibitors to the 30 active site of HDLP to ascertain how well the shape and the

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structure of the potential inhibitor complement the active site or to compare the potential inhibitors with the binding of TSA or SAHA in the active See Bugg et al, 1998, Scientific American December:92-98; West et al., 1995, TIPS <u>16</u>:67-74. potential inhibitors designed by modeling with a docking program conform to the general formula (I) as described Computer programs may also be employed to estimate the attraction, repulsion and stearic hindrance of the HDLP and potential inhibitor compound. Generally, the tighter the fit, the lower the stearic hindrances, the greater the attractive forces, and the greater the specificity which are important features for a specific inhibitory compound which is more likely to interact with HDLP and HDLP-related proteins rather than other classes of proteins. These features are desired particularly where the inhibitory compound is a potential antitumor drug.

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The compounds of the present invention may also be designed by visually inspecting the three-dimensional structure to 20 determine more effective deacetylase inhibitors. This type of modeling may be referred to as "manual" drug design. Manual drug design may employ visual inspection and analysis using a graphics visualization program such as "0" (Jones, T.A., Zhou, J.Y., Cowan, S.W., and Kjeldgaard, M., Improved 25 method for building protein models in electron density maps the location of errors in these models, Acta Crystallog., A47, 110-119.

Initially potential inhibitor compounds can be selected for their structural similarity to the X, Y and Z constituents

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of formula (I) by manual drug design. The structural analog thus designed can then be modified by computer modeling programs to better define the most likely effective candidates. Reduction of the number of potential candidates is useful as it may not be possible to synthesize and screen a countless number of variations compounds that may have some similarity to known inhibitory molecules. Such analysis has been shown effective in the development of HIV protease inhibitors (Lam et al., 1994, Science 263:380-384; Wlodawer et al., 1993, Ann. Rev. Biochem. <u>62</u>:543-585; Appelt, 1993 Perspectives in Drug Discovery and Design 1:23-48; Erickson, 1993, Perspectives in Drug Discovery and Alternatively, random screening of an Design <u>1</u>:109-128. small molecule library could lead to potential inhibitors whose inhibitory activity may then be analyzed by computer modeling as described above to better determine their effectiveness as inhibitors.

The compounds designed using the information of the present invention may be competitive or noncompetitive inhibitors. These designed inhibitors may bind to all or a portion of the active site of HDLP and may be more potent, more toxic and more effective than known specific, less HDLP-related proteins, HDLP and for inhibitors The designed inhibitors may also be particularly HDACs. less potent but have a longer half life in vivo and/or in vitro and therefore be more effective at inhibiting histone deacetylase activity in vivo and/or in vivo for prolonged Said designed inhibitors are useful to periods of time. inhibit the histone deacetylase activity of HDLP and HDLPrelated proteins (e.g. HDAC1), to inhibit cell growth in

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vitro and in vivo and may be particularly useful as antitumor agents.

The present invention also permits the use of molecular design techniques to computationally screen small molecule data bases for chemical entities or compounds that can bind to HDLP in a manner analogous to the TSA and SAHA as defined by the structure of the present invention. computational screening may identify various groups which may be defined as "X", "Y" or "Z" of formula (I) above and may be employed to synthesize the potential inhibitors of the present invention comprising formula (I). Such potential inhibitors may be assayed for histone deacetylase inhibitory activity in a histone deacetylase activity assay (see Example 3 below), may be co-crystallized with HDLP to determine the binding characteristics through X-ray crystallography techniques defined above (e.g. said cocrystal structure may be determined by molecular replacement to assess the binding characteristics of said potential inhibitor), or may be assessed based on binding activity by incubating said potential inhibitor with said HDLP, performing gel filtration to separate any free potential inhibitor to HDLP-bound inhibitor, and determining the amount of histone deacetylase activity of the inhibitorbound HDLP. To measure binding constants (e.g., Kd), methods known to those in the art may be employed such as $\operatorname{Biacore}^{\operatorname{m}}$ analysis, isothermal titration calorimetry, Elisa with a known drug on the plate to show competitive binding, or by a deacetylase activity assay.

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The design of potential inhibitors of the present invention is further facilitated by reference to Figure 9, which is a surface representation figure that depicts the surface grooves. Analysis of such grooves gives insight into the constituents of the cap group of formula (I). grooves are labeled groove A, groove A', groove B and groove C, into which additional cap groups may bind. The structure of HDLP bound to either TSA or SAHA shows that the cap groups of TSA and SAHA bind in groove A. By analysis of the amino acid sequence identity of HDLP and HDACs, Groove A is well conserved in HDACs, has a significant hydrophobic component, appears deep enough to allow for significant interactions and is also the largest of the four grooves. In addition to the dimethylamino phenyl group of the TSA, the A groove can fit approximately 200 daltons worth of groups (e.g. groove A could accommodate a naphthalene-like group after an appropriate spacer, etc.). Groove A, as referred to herein, is characterized by the following conserved residues of HDLP: His 21, Pro22, Lys24, Phe141, Leu265 and Phe335. The periphery of groove A comprises unconserved residues. Additionally, Groove A', as referred to herein, comprises primarily unconserved residues.

Groove B is immediately adjacent to the pocket. Of significance is that the bottom of groove B comprises the N-epsilon nitrogen of His170, which coordinates the zinc through its N-delta nitrogen. Significant binding energy may be achieved by contacting the Ne proton of His170 with a carboxylic acid or sulfate group. In addition, groove B may be large enough to fit a phenyl group, the face of which may comprise a partial negative charge which may pack over the N-epsilon proton of His170. The conserved residues of

- 44 ~

groove B, as referred to herein are: His170, Tyr196 and Leu265.

Groove C is not as well conserved as the other two grooves and the amino acid residues which comprise groove C are mostly polar and solvent exposed. Groove C, as referred to herein comprises the following conserved residues: Asn87, Gly140 and Phe198.

The compounds of the present invention are represented by formula (I):

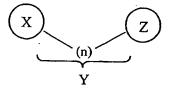
(I)

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Examples for suitable X constituents wherein X comprises a cap group may be described in three categories, depending upon which surface of groove A, A', B and/or C they are targeted to. The cap group may comprise all three categories on the same compound. Of particular benefit may be replacing the cap group of TSA or SAHA with a large, rigid structure. Nonlimiting examples for suitable cap groups (X) of formula (I) which may bind in groove A are: (1) attaching a 1-3 methyl linker followed by a phenyl or naphthalene group from the para or meta position of SAHA's phenyl group represented by formula (IV):

(IV)

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(2) attaching a 2-3 methyl linker followed by a phenyl or naphthalene group from the meta position of TSA's phenyl cap group, or from TSA's dimethyl amino group represented by formula (V):

(V)

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and which may bind in groove B is a 1-3 methyl group spacer followed by a carboxylate, sulfate or phenyl group as represented by formula (VI):

(VI)

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With respect to the aliphatic (Y) group, the diameter of the pocket suggests that one more methyl "side chain" could fit, in addition to the C15 methyl group on the C10 carbon. Nonlimiting suitable examples for Y constituents wherein Y comprises an aliphatic chain group are as follows: (1) add

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a methyl group to TSA on the C12 carbon (with or without a methyl group on the C10 carbon and with or without double bonds and with or without substituting the X and/or Z constituents of formula (I)as represented by formula (VII):

(VII)

(branch here) - 8 (15)

10 (2) add a methyl group to TSA on the C9 carbon (with or without a methyl group on the C10 carbon; with or without both or either of the double bonds, and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VIII):

(VIII)

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(3) replace the two alkalene double bonds of TSA with only one between C10 and C11, which may free the C11 and C12 torsion to allow for a better fit, the X and/or Z groups may also be substituted as represented by formula (IX):

25 (IX)

(4) cyclize C15 and C12 carbons of TSA through a sulphur atom (or nitrogen atom), the X and/or Z groups may also be substituted as represented by formula (X):

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(5) extend from the C9 carbon of TSA such that the extension approaches and/or enters groove B (see Figure 9); making C9 sp3 so that it can have some freedom; attach to C9 a 1-3 methyl group spacer which may include a double bond and they attaching thereto a sulfate, carboxylate, sulfate, hyroxyl, or phenyl group which may make an interaction with the N-epsilon proton of His170 which may coordinate the zinc atom as represented by formula (XI):

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$$X \longrightarrow \begin{cases} (16) \\ (16) \\ (2) \\ (CH_2)n \\ R_1 \end{cases}$$

25 (6) extend off the C8 carbon (replacing C14) of TSA such that the extension approaches or enters groove B; attach a 1-3 methyl group spacer (which may include a double bond) and then link thereto a carboxylate, sulfate, hydroxyl or phenyl group such that an interaction is made with the N-epsilon proton of His170 that coordinates the zinc atom; the X and/or Z constituents may also be substituted as represented by formula (XII):

(XII)

$$\begin{array}{c|c} R_1 \\ (CH_2)n & (_{15}) \\ \hline \\ X \end{array} \begin{array}{c} R_1 \\ COOH \\ SO_4 \\ OH \end{array}$$

(7) substitute the C8 carbon at the end of the aliphatic chain such that the substitution may contact groove A, A', B and or C, in such an example, a cap group (X) may or may not be required and the X and Z constituents may be substituted as well, as represented by formula (XIII):

(XIII)

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(8) formulas VII through XIII above wherein the aliphatic chain further comprises a methyl group between the active site binding group (Z) and the C8 carbon, and preferably just before the C8 carbon, increasing the distance between X and Z, (9) make the connection between the aliphatic chain and the cap group more rigid (e.g., by closing a 6-membered ring which may or may not comprise oxygen, the X and Z group may also be substituted as represented by formula (XIV):

(XIV)

and (10) combining two or more of the changes depicted by formulas (VII-XIV).

Additionally, nonlimiting examples for suitable Z groups wherein Z comprises an active site binding group are as follows: (1) hydroxamic acid, (2) carboxylic acid, (3) sulfonamide, (4) acetamide, (5) epoxyketone, (6) an ester with a methyl linker and a hydroxyl of acetate ester group to lead into the cavity and interact with a conserved arginine (Arg27) as represented by formula (XV): (XV)

$$R_1$$
 CH_2 R_1 CH_2 R_1 R_1 R_2 R_3 R_4 R_4 R_5 R_6 $R_$

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and (7) an alphaketone as represented by formula (XVI): (IVX)

$$R_{1} = \begin{cases} --(CH_{2})n - OH \\ --(CH_{2})n - C \\ --(CH_{2})n - C \\ O - CH_{3} \end{cases}$$

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Additionally, other suitable X, Y and Z constituents may be the skilled artisan given the threeenvisioned by dimensional structural information of the present invention.

After having determined potential suitable X, Y and Z constituents, the constituents are combined to form a compound of formula (I) using combinatorial chemistry techniques. This may be achieved according to U.S. Patent 5,700,811; 5,773,474; 5,840,960 5,608,108; 5,668,179, incorporated herein by reference. Any methods

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known to one of skill in the art may be employed to synthesize compounds of formula (I) comprising X, Y and Z constituents as determined by the methods described above.

As mentioned above, the compounds of formula (I) are useful to inhibit the histone deacetylase activity of HDLP and HDAC-related proteins. Such inhibition may allow for a reduction or cessation of cell growth in vitro and in vivo.

For in vitro use, such reduction or cessation of cell growth 10 is useful to study the role of histone deacetylation and differentiation during the cell cycle and also to study other mechanisms associated with cell cycle arrest and particularly how the repression of transcription is involved in cell cycle progression which may be studies in a yeast 15 model system such as that described by Kadosh & Struhl, 1998, Mol. Cell. Biol. <u>18</u>:5121-5127. In vitro model systems which may be employed to study the effects of potential inhibitors on cell cycle progression and also tumor growth include those described by: Richon et al, 1998, Proc. Natl. 20 Acad. Sci. USA <u>95</u>:3003-3007; Yoshida et al., 1995, Bioessays 17:423-430; Kim et al., 1999, Oncogene 18:2461-2470; Richon et al., 1996, Proc. Natl. Acad. Sci. USA 93:5705-5708; and Yoshida et al., 1987, Cancer Res. 47:3688-3691.

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For in vivo use, such a reduction or cessation of cell growth is useful to study the effect of said inhibitor compounds in non-human animal model systems of cancer and is also useful for the treatment of cancer in a recipient in need of such treatment. Non-limiting examples of animals which may serve as non-human animal model systems include

mice, rats, rabbits, chickens, sheep, goats, cows, pigs, and non-human primates. See, e.g., Desai et al., 1999, Proc. AACR 40: abstract #2396; Cohen et al., 1999, Cancer Res., submitted. The compounds of the present invention may be administered to a transgenic non-human animal wherein said animal has developed cancer such as those animal models in which the animal has a propensity for developing cancer (e.g. animal model systems described in U.S. Patents 5,777,193, 5,811,634, 5,709,844, 5,698,764, and 5,550,316). Such animal model systems may allow for the determination of toxicity and tumor reduction effectiveness of the compounds of the present invention.

A preferred compound of the present invention may comprise high specific activity for HDLP and HDAC-related proteins, good bioavailability when administered orally, activity in reducing or ceasing cell growth in tumor cell lines, and activity in reducing or ceasing tumor growth in animal models of various cancers.

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Accordingly, another aspect of this invention is a method of eradicating or managing cancer in a recipient, which may be an animal and is preferably a human. Said method comprises administering to said recipient a tumor reducing amount of a compound as defined by formula (I) above, or a physiological acceptable salt thereof.

In a further aspect of the invention, there is provided a composition comprising the compound of formula (I) and an excipient or carrier. Administration of the foregoing agents may be local or systemic. Such carriers include any

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suitable physiological solutions or dispersant or the like. The physiologic solutions include any acceptable solution or dispersion media, such as saline, or buffered saline. The carrier may also include antibacterial and antifungal agents, isotonic and absorption delaying agents, and the like. Except insofar as any conventional media, carrier or agent is incompatible with the active ingredient, its use in the compositions is contemplated.

- Routes of administration for the compositions containing the 10 delivery vehicle constructs of the present invention include any conventional and physiologically acceptable routes, such as, for example, oral, pulmonary, parenteral (intramuscular, intraperitoneal, intravenous (IV) or subcutaneous injection), inhalation (via a fine powder formulation or a 15 mist), transdermal, nasal, vaginal, rectal, sublingual routes of administration and can be formulated in dosage forms appropriate for each route of administration.
- The following examples are provided to more clearly illustrate the aspects of the invention and are not intended to limit the scope of the invention.

EXAMPLES

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25 Example 1: Protein Production and Purification:

Full-length wild-type HDLP (Genbank accession number AE000719) was subcloned from an Aquifex aeolicus chromosomal DNA preparation (provided by Robert Huber of Universitaet of Regensburg, Germany) into the pGEX4T3 (Amersham-Pharmacia, Piscataway, NJ) vector using the polymerase chain reaction (PCR). The cysteine-to-serine and active site mutants were constructed by PCR site directed mutagenesis and were

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sequenced. The HDLP-glutathione S-transferase (GST) fusion protein was produced in Escherichia coli, purified by column a chromatography using affinity glutathione-sepharose resin (Amersham-Pharmacia, Piscataway, NJ), and by anion-exchange chromatography (Q-sepharose $^{\mathbf{m}}$; Amersham-Pharmacia, Piscataway, NJ). HDLP was cleaved from the fusion protein with thrombin at 4° C, was purified by Amersham-Pharmacia, (Q-sepharose™; anion-exchange filtration chromatography gel and (LN Piscataway, (Superdex™200; Amersham-Pharmacia, Piscataway, NJ), and was concentrated to typically 25 mg/ml in a buffer of 25 mM bis-tris propane (BTP), 500 mM NaCl, 5 mM dithiothrietiol (DTT), 2% isopropanol, pH 7.0.

Although, it is not known what metal cofactor HDLP contains 15 in vivo, it is presumed to be zinc because of arrangement of the ligands and the similarities in the active site to the zinc proteases. The lack of metal in the purified HDLP is presumed due, in part, to the use of DTT during purification. HDLP was reconstituted with Zn^{2+} by 20 mixing the Cys75Ser/Cys77Ser double mutant at 10 mg/ml with a 5-fold molar excess of ${\rm ZnCl_2}$ in a buffer of 25 mM bis-tris propane, 200 mM NaCl, 1% isopropanol, pH 7.0. Unbound ZnCl2 was removed by fractionating HDLP through a G25 desalting Piscataway, NJ). The (Amersham-Pharmacia, 25 column $\mathtt{HDLP-Zn^{2+}-TSA}$ complex was prepared by incubating the $\mathtt{Zn^{2+}}$ reconstituted HDLP mutant with 1 mM TSA for 45 minutes, followed by gel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ) to remove excess TSA, and concentration to typically 25 mg/ml in a buffer of 25 mM $\,$ 30 bis-tris propane, 500 mM NaCl, 1% isopropanol, pH 7.0.

FLAG epitope tagged human HDAC1 was overexpressed using a baculovirus expression system in Hi5 (Invitrogen, Carlsbad, CA) insect cells grown in suspension in serum-free media (Sf900, Gibco, Grand Island, NY). The fusion protein was purified by anion exchange and affinity chromatography using Anti-FLAG M2 affinity resin (Sigma, St. Louis, MO) and FLAG Peptide (Sigma,, St. Louis, MO).

Example 2: Crystallization and data collection:

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10 Crystals of apo-HDLP were grown at room temperature by the hanging-drop vapor-diffusion method, from 7.5% isopropanol, 28% PEG 1500, 425 mM NaCl, 100 mM Tris-Cl, pH 7.0. They form in space group C2 with a = 51.4 Å, b = 93.8 Å, c = 78.7 Å, β = 96.9 Å, and contain one HDLP molecule in the asymmetric unit. Diffraction data were collected with crystals flash-frozen in a buffer of 7.5% isopropanol, 35% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, at -170° C.

The structure of the HDLP- Zn²+ complex was determined from HDLP Cys75Ser/Cys77Ser double mutant crystals grown from 23% tert-butanol, 27% PEG 1500, 400 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8. Space group and cell dimensions were identical to the apocrystals. The HDLP-Zn²+ crystals were harvested and frozen in 27% tert-butanol, 22% PEG 1500, 50 mM KCl, 20 mM NaCl, 0.2 mM ZnCl₂, 100 mM bis-tris propane, pH 6.8, at -170° C.

Crystals of the HDLP-Zn²⁺-TSA complex comprised HDLP Cys75Ser/Cys77Ser double mutant and were grown from 23% tert-butanol, 27% PEG 1500, 600 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8, by microseeding. The crystals were grown in the presence of zinc. They form in space group

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 $P2_12_12_1$ with a = 53.4 Å, b = 94.4 Å, c = 156.3 Å and contain two HDLP- Zn^{2+} -TSA complexes in the asymmetric unit. The HDLP- Zn^{2+} -TSA crystals were harvested and frozen in the same cryobuffer as the HDLP- Zn^{2+} crystals except that 0.5mM TSA was added. Data were processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, Method. Ensemble. 276:307-326). MIR analysis, model building and refinement.

The HDLP-Zn²⁺-SAHA complex crystals were grown and evaluated the same as the HDLP-Zn²⁺-TSA crystals. However, the restraints for the SAHA structure were constructed based on stereochemical parameters from TSA. Like the apo-HDLP crystals, the SAHA/HDLP co-crystals grew in space group C2.

Heavy-atom soaks were performed with the apo-HDLP crystals 15 in a buffer of 7.5% isopropanol, 30% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, supplemented with 1.0 mM thimerosal for 2h, 5 mM $KAu(CN)_2$ for 1h, and 1 mM $Pb(Me)_3OAc$ for 2h. MIR phases were calculated with the program MLPHARE (The CCP4 suite: Programs for computational crystallography, 20 1994, Acta Crystallogr. D <u>50</u>:760-763) at 2.5 Å using the anomalous diffraction signal from the thimerosal derivative, and had a mean figure of merit of 0.55. The phases were improved by solvent flattening with the program DM (The CCP4 suite: Programs for computational crystallography, 1994, 25 Acta Crystallogr. D 50:760-763) , and were used to build the initial model with the program O (Jones et al., 1991, Acta Crystallogr. A 47:110-109). Successive rounds of rebuilding and simulated annealing refinement with the program CNS (Brunger et al., 1998, Acta Crystallogr. D 30 54:905-921) allowed interpretation of HDLP from residues 2

to 373. Residues 1, 374, and 375 were not modeled and are presumed to be disordered.

The structure of the $HDLP-Zn^{2+}-TSA$ and $HDLP-Zn^{2+}-SAHA$ complex were determined by molecular replacement with the program 5 suite: Programs for computational AMORE (The CCP4 crystallography, 1994, Acta Crystallogr. D 50:760-763) using the apo-HDLP structure as a search model. The initial electron density maps had strong and continuous difference density for the entire TSA molecule. However the SAHA molecule was not as well ordered in the cap group region. The structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST) and was used to define stereochemical restraints used in the refinement with the program CNS. The restraints of SAHA were constructed based on stereochemical parameters from TSA and surrounding amino acid residues. The dimer interface in the HDLP-Zn2+-TSA and $\mbox{HDLP-Zn}^{2+}\mbox{-SAHA}$ crystals primarily involves Phe200 on the protein surface. The Phe200 side chain contacts Tyr91, whose side chain conformation changes on TSA binding, and part of the dimethyl amino phenyl group of TSA from the second protomer. The HDAC family does not contain a phenylalanine residue at the equivalent position.

25 Example 3: Histone deacetylase assays:

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Purified proteins were assayed by incubating 10 μg of [3H] acetyl-labeled murine erythroleukemia histone substrate and HDAC assay buffer (20 mM Tris-HCl, pH 8.0, 150 mM NaCl, 10% glycerol) for 30-60 minutes at 37° C in a total volume of 30 μ l. The final concentrations of HDLP and HDACl-FLAG were 3.6 μ M and 0.24 μ M, respectively. Assays were performed in duplicate. The reactions were stopped and the

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released acetate was extracted and assayed as described (Hendzel et al., 1991, J. Biol. Chem. 266:21936-21942). [3H] acetyl-labeled murine erythroleukemia histones were prepared essentially as described (Carmen et al., 1996, J. Biol. Chem. 271:15837-15844). Inhibitors were added in the absence of substrate and incubated on ice for 20 minutes, substrate was added, and the assay performed as described above. HDLP was inclubated with 20 μ M ZnCl₂ and 20 μ M MnCl₂(H2O)₄ in HDAC buffer and tested for activity.

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Only HDLP dialyzed against ${\rm ZnCl_2}$ had activity. HDAC1-FLAG was dialyzed against 20 μM ${\rm ZnCl_2}$ in HDAC buffer which had no effect on activity. Therefore, HDAC1-FLAG contains a metal as purified.

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The in vivo substrate of HDLP is not known. HDLP may have a role in acetoin utilization like the B. subtilis AcuC gene product, and it has been annotated as such in the genome sequence, but the reaction catalyzed by AcuC is also not known. Furthermore, the A. aeolicus genome appears to lack the acuA and acuB genes that are part of the acuABC operon of B. subtilis (Deckert et al., 1998 Nature 392:353-358), and HDLP is as similar to human HDAC1 (35.2 % identity) as it is to B. subtilis AcuC (34.7 % identity).

What is claimed is:

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- A crystal of an enzyme comprising deacetylase activity 1. wherein said crystal effectively diffracts X-rays for the determination of the atomic coordinates of said 5 enzyme to a resolution of greater than 4 Å and wherein the structure of said enzyme comprises a conserved core α/β structure characteristic fold wherein said conserved α/β fold comprises an eight-stranded parallel 10 eta sheet and eight lpha helices and wherein four of the helices pack on either face of said parallel β sheet and wherein said structure of said enzyme comprises an rmsd of less than or equal to 1.5 Å in the positions of $C\alpha$ atoms for at least 2/3 or more of the amino acids of 15 HDLP as defined by the atomic coordinates of HDLP.
 - 2. The crystal of claim 1, wherein said protein structure further comprises:
 - (a) eight α helices positioned near one side of the β sheet; and
 - (b) at least seven large, well defined loops originating from the C-terminal ends of the β -strands of said eight-stranded parallel β sheet wherein the eight extra helices and the seven large loops are associated with a significant extension of the structure beyond the core α/β motif and wherein said extension of the structure gives rise to a deep, narrow pocket and an internal cavity adjacent to the pocket.

3. The crystal of claim 1, wherein said enzyme comprising deacetylase activity is selected from the group

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consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, AcuC, and functional derivatives thereof.

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- 4. The crystal of claim 2 further comprising a specifically bound zinc atom in the active site of said enzyme.
- 10 5. The crystal of claim 2 further comprising a specifically bound deacetylase inhibitor compound in the active site of said enzyme.
- 6. The crystal of claim 2 define by the atomic coordinates according to Figure 16.
 - 7. A method for identifying a potential deacetylase inhibitor compound for an enzyme which comprises deacetylase activity, said method comprising the steps of:
 - using a three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16;
 - employing said three-dimensional structure to design or select said potential inhibitor;
 - c. synthesizing said potential inhibitor;
 - d. contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate;
 and
- e. determining the deacetylase inhibitory activity of said potential inhibitor.

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8. The method of claim 7, wherein the three-dimensional structure is designed or selected using computer modeling.

- 5 9. The method of claim 7, wherein the potential deacetylase inhibitor is designed de novo.
- 10. The method of claim 7, wherein the potential deacetylase inhibitor is designed based on a known inhibitor.
- 11. The method of claim 7, wherein said enzyme comprising deacetylase activity is selected from the group consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, and AcuC.
- 12. A method of evaluating the binding properties of the potential deacetylase inhibitor compound comprising the steps of:
 - a. co-crystallizing said compound with HDLP;

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- b. determining the three-dimensional structure of said HDLP-potential inhibitor complex co-crystal by molecular replacement using the threedimensional structure of HDLP as defined by atomic coordinates according to Figure 16; and
- c. analyzing said three-dimensional structure of said HDLP bound to said potential inhibitor compound to evaluate the binding characteristics of said potential inhibitor compound.
- 13. A method for solving the structure of an HDAC family

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member crystal comprising the steps of:

- a. collecting X-ray diffraction data of said crystal wherein said data diffracts to a high resolution limit of greater than 4 Å;
- b. using the atomic coordinates of HDLP accoding to Figure 16 to perform molecular replacement or refinement and difference fourier with said X-ray diffraction data of said HDAC family member crystal to determine the structure of said HDAC family member; and
- c. refining said structure of said HDAC family member.
- 14. The method of claim 13, wherein said HDAC family member is HDAC1.
 - 15. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant is encoded by the nucleic acid sequence of SEQ ID NO:4.
 - 16. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant has the amino acid sequence of SEQ ID NO:3.
 - 17. A nucleotide sequence according to SEQ ID NO:4
 - 18. An expression vector comprising the nucleotide sequence of claim 17.
- 19. A method of using the crystal of claim 1 for screening30 for a novel drug comprising:
 - a. selecting a potential ligand by performing

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rational drug design with the three-dimensional structure determined for the crystal;

- b. contacting the potential ligand with the ligand
 binding domain of the crystal; and
- c. detecting the binding potential of the potential ligand for the ligand binding domain, wherein the novel drug is selected based on its having a greater affinity for the ligand binding domain than that of a known drug.

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Statistics from the crystallographic analysis

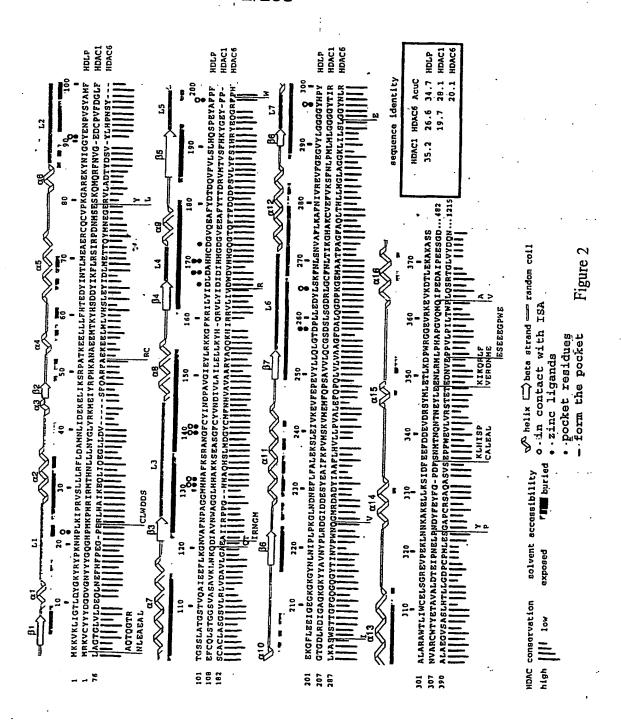
TABLE 1.

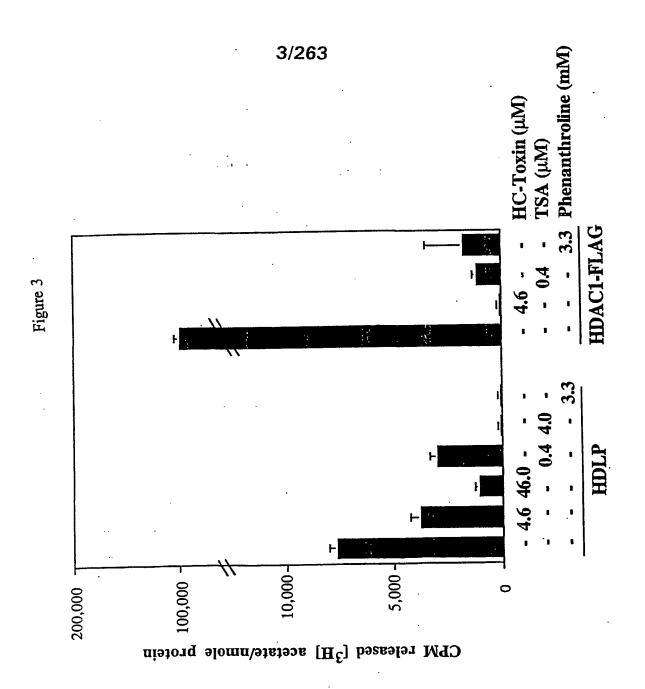
1/263

| Data set | | Native | thimerosal | Pb | Aucn | Zu | TSA | | |
|--|--------------------------------|---|--|---|---|---|---|--------------|--|
| Space Group Resolution (Å) Observations Unique reflections Data coverage (%) Rsym (%) MIR analysis (20.0-2.5 Å): phasing power Rcullis Rcullis (ano) | 2.5 A): | C2 1.8 134,952 32,143 92.3 2.9 | C2 2.3 79,023 15,958 95.7 8.4 1.47 0.72 | C2 3.5 11,454 4,040 86.4 9.6 1.24 0.78 | C2 2.8 27,722 8,753 94.3 8.9 1.10 | C2 2.0 125,769 23,643 90.6 7.2 | P2,2,2,1 2.1 180,427 50,796 93.8 7.1 | | |
| Refinement statistics | ;; | | | | | - | RMSD | | |
| Data Resoluti Set (Å) | tion Reflections (IFI > 10) | ns Total s) atoms | u Water ns atoms | R-factor (%) | R-free (%) | bonds (Å) | angles (°) | B-factor (Ų) | |
| HDLP 1.8 | 31,550 | | | | 24.0 | 0.010 | 1.63 | 3.55 | |
| HDLP-Zn 2.0. | 23,582 | | | 22.0 | 25.8 | 0.009 | 1.48 | 1.04 | |
| HDLP-Zn-TSA 2.1. | 44,122 | | | 22.4 | 25.8 | 0.008 | 1.78 | 3.83 | |
| | | | | | | | | - | |

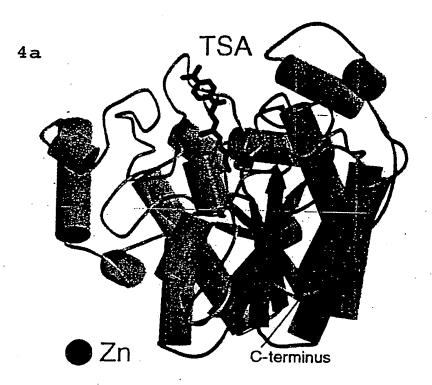
 $\mathsf{F}_{\mathsf{calc}}$ $|/\Sigma|\mathsf{F}_{\mathsf{obs}}$, where $\mathsf{F}_{\mathsf{obs}}$ and $\mathsf{F}_{\mathsf{calc}}$ are the observed and calculated structure factors, respectively. Figure of merit = IF(hkl)best[/F(hkl). R-free = R-factor calculated using 5% of the reflection data chosen randomly and omitted from the start of refinement. RMSD: root mean square deviations from ideal geometry and root Rsym = $\Sigma_h \Sigma_l$ II_{h,l}-<l_h|>/ $\Sigma_h \Sigma_l$ I_{h,l} for the intensity (I) of i observations of reflection h. Phasing power = <F_{λl >/E,} where $<F_{\lambda l}>$ is the root-mean-square heavy atom structure factor and E is the residual lack of closure error. Rcullis is the mean residual lack of closure error divided by the dispersive difference. R-factor = Σ l $F_{
m obs}$ mean square variation in the B-factor of bonded atoms.











4b

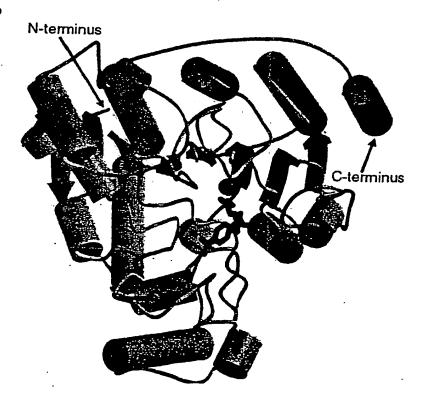
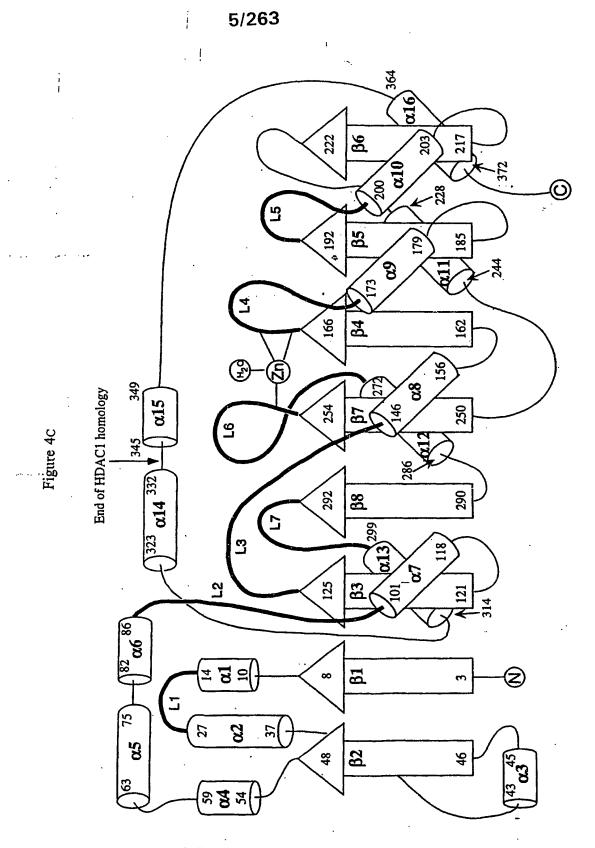


Figure 4
SUBSTITUTE SHEET (RULE 26)



SUBSTITUTE SHEET (RULE 26)

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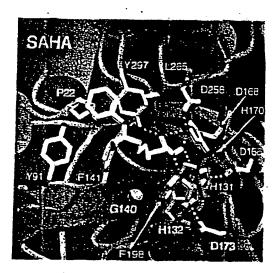
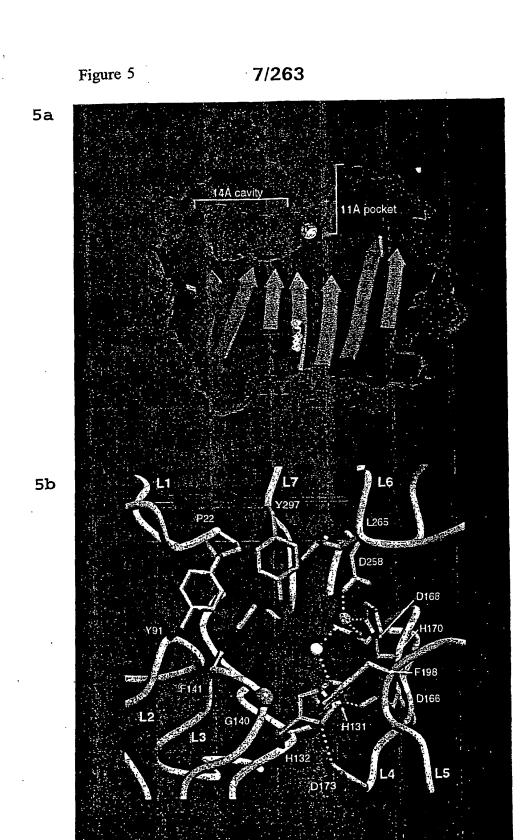


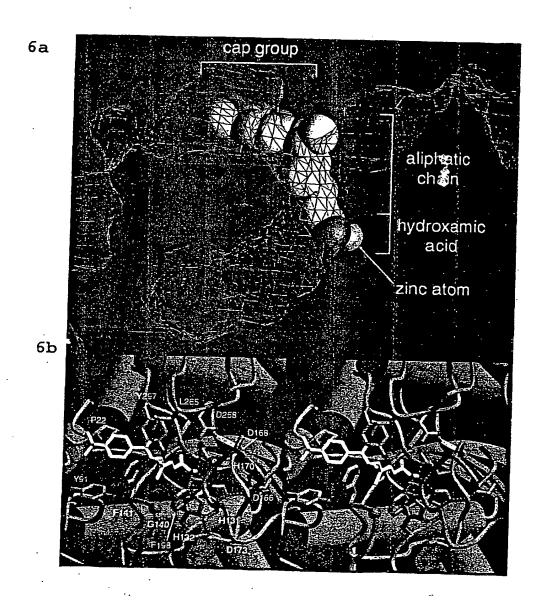
Figure 4D



SUBSTITUTE SHEET (RULE 26)

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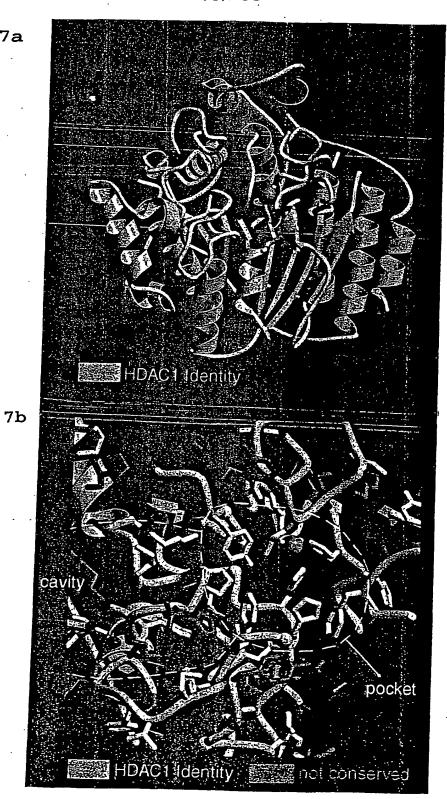
Figure 6



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Figure 7

7a



SUBSTITUTE SHEET (RULE 26)

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SUBSTITUTE SHEET (RULE 26)

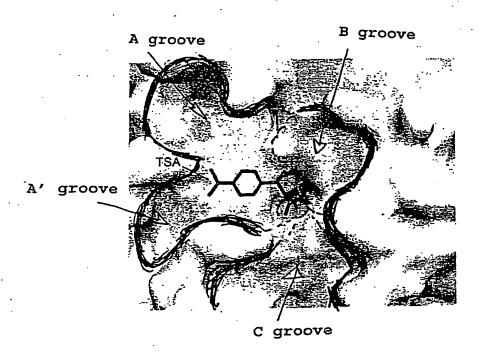
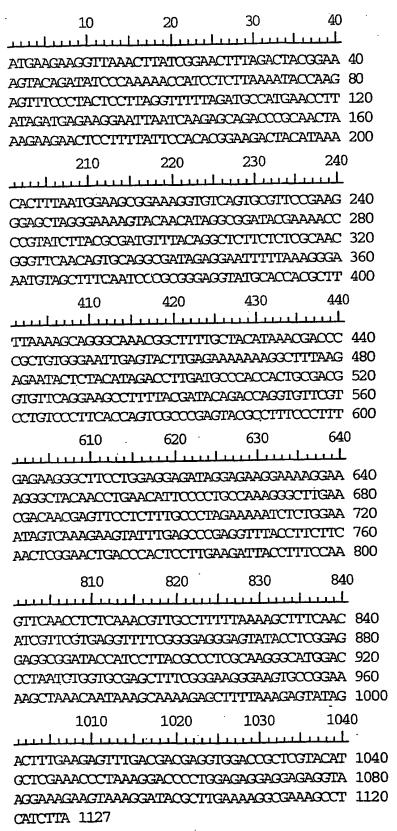


Figure 9

Figure 10

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SUBSTITUTE SHEET (RULE 26)

Figure 11

| ٠. | . 10 . | 20 | 30 | 40 | |
|---------|------------|-----------|------------|--------|-----|
| بليبيد | بليسلين | بتتبليين | سيطييي | huul | |
| MKKVKL | IGTLDYGKYF | XYPKNHPLK | IPRVSLLLRF | LDAMNL | 40 |
| IDEKEL | IKSRPATKEE | LLLFHTED | YINTIMEAER | CQCVPK | 80 |
| GAREKY | NIGGYENPVS | YAMFIGSS | LATGSTVQAI | EEFLKG | 120 |
| NVAFNP | AGGMHHAFKS | RANGFCYI | NDPAVGIEYL | RKKGFK | 160 |
| RILYID | LDAHHCDGVQ | EAFYDTDC | VFVLSLHQSP | EYAFPF | 200 |
| | 210 | 220 | 230 | 240 |) |
| بليبيد | ىلىنىلىن | سيليب | سيطينيا | لمسل | |
| EKGFLE | EIGEGKGKGY | NLNIPLPK | GLNDNEFLFA | LEKSLE | 240 |
| IVKEVF | EPEVYLLQLO | FIDPLLEDY | LSKFNLSNVA | FLKAFN | 280 |
| | | | AWILIWCELS | | |
| KLNNKA | KELLKSIDFF | EFDDEVDF | SYMLETLKDF | WRGGEV | 360 |
| רוש פשם | TEKAKASS | 375 | | | |

Figure 12

| | _ | | |
|------------------|-------------|---|------------------|
| 10 | 20 | 30 | 40 |
| | | لتتتليبيا | لبيا |
| ATGAAGAAGGITAAA | CTTATCGGA | ACTITAGACTA | CGGAA 40 |
| AGTACAGATATCCCA | | | |
| AGTITICCCTACTCCT | | | |
| ATAGATGAGAAGGAA | | | |
| AAGAAGAACTCCTT | | | |
| 210 | 220 | 230 | 240 |
| | | لتتبايينا | |
| CACTITAATGGAAGC | | | |
| GGAGCTAGGGAAAA | | | |
| CCGTATCTTACGCG | | | |
| GGGTTCAACAGTGC | | | |
| AATGTAGCTTTCAAT | | | |
| 410 | 420 | 430 | 440 |
| | | 1,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | لبييا |
| TTAAAAGCAGGCA | | | |
| CCTCTCCCAATTC | | | |
| AGAATACTCTACAT | | | |
| GIGITICAGGAAGCC | | | |
| CCTGTCCCTTCACC | | | |
| 610 | 620 | 630 | 640 _. |
| <u></u> | سيلسيا | سيلسن | |
| GAGAAGGGCTTCCT | GAGGAGATZ | AGGAGAAGGAA | AAGGAA 640 |
| AGGGCTACAACCTG | | | |
| CGACAACGAGTICC | ICTITGCCCT | TAGAAAATCT | CIGGAA 720 |
| ATAGTCAAAGAAGT | | | |
| AACTCGGAACTGAC | CCACTCCTT | SAAGATTACCT | TICCAA 800 |
| 810 | 820 | 830 | 840 |
| | | | ا ا |
| GTTCAACCTCTCAAA | بالككالياتك | TTTAAAAGCTT | TICAAC 840 |
| ATCGTTCGTGAGGTT | | | |
| GAGGCGGATTCCATC | | | |
| CCTAATCTGGTGCGA | | | |
| AAGCTAAACAATAAA | | | |
| 1010 | 1020 | 1030 | 1040 |
| | | 1050 Liilii | |
| ACTITGAAGAGTITG | | | |
| GCTCGAAACCCTAAA | | | |
| AGGAAAGAAGTAAAG | | | |
| CATCITA 1127 | | • | |
| | 200211 | TUTE SHEET | (MULL 26) |

Figure 13

| | 10 | 20 | 30 | 40 | |
|-------------------------------|---------------------------------|-------------------------------------|--------------------------|--|---|
| بيلينين | ليتنجلين | malia. | سسلسسا | بليييا | |
| MKKVKLI | GTLDYGKY | RYPKNHPLK | IPRVSLLLRF | LDAMNL 40 | |
| IDEKELI | KSRPATKE | ELLLFHTED | YINILMEAER | CQCVPK 80 | |
| GAREKYN | IIGGYENPV | SYAMFIGSS | LATGSTVQAT | EEFLKG 12 | 0 |
| NVAFNPA | GGMHHAFK | SRANGFCYL | NDPAVGIEYL | RKKGFK 16 | 0 |
| RILYIDL | DAHHCDGV | QEAFYDIDQ | VFVLSLHQSP | EYAFPF 20 | 0 |
| | 04.0 | | | | |
| | 210 | . 220 | 230 | 240 | |
| تتلييي | | . 220 | | | |
| | لسلب | سسلسب | | لسبل | 0 |
| EKGFLEE | IGEGKGKG | YNLNIPLPK | سيلسن | LUUL LEKSLE 24 | _ |
| EKGFLEE IVKEVFE | DEVATTÓT TŒEŒKŒKŒ | GIDPLLEDY | GINDNEFLFA | LEKSLE 24 FLKAFN 28 | 0 |
| EKGFLEE IVKEVFE IVREVFG | IGEGKGKG PEVYLLQL EGVYLGG | YNLNIPLPK GIDPLLEDY GFHPYALAR | LINDNEFLFA LSKFNLSNVA | LLLLL LEKSLE 24 FLKAFN 28 GREVPE 32 | 0 |

17/263 Figure 14

| 10 | 20 | 30 | 40 |
|--------------------------------------|----------------------------|---|-------------------|
| اسالسالى | ليتبيلين | لتسليين | سب |
| ATGAAGAAGGTTAAAC | | | |
| AGTACAGATATCCCAA | | | |
| AGITICCCTACICCTT | | | |
| ATAGATGAGAAGGAAT | | | |
| AAGAAGAACTCCTTTT | | | |
| 210 | 220 | 230 | 240 |
| 210 | | | |
| CACTITAATGGAAGCG | | | |
| GGAGCTAGGGAAAAGI | | | |
| CCGTATCTTACGCGAT | | | |
| GGGTTCAACAGTGCAG | KOLCDUDUDU KOLCDUDUDUDU | ΔΑΤΉΤΗΝΑΔΩΣ ΑΑΤΉΤΗΝΑΔΩΣ | AGGGA 360 |
| AATGTAGCTTTCAATC | | | |
| • | | 430 | 440 |
| 410 | 420 | | - |
| | ~~~~ | \sim | 22CC 440 |
| TTAAAAGCAGGCAAA | ADSCALLES CO. | 2 | 7772 AG 480 |
| CGCIGIGGGAATTGAC AGAATACTCTACATAC | | ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ | 77°230°2 520 |
| AGAATACICTACATAC | | | |
| CCTGTCCCTTCACCAC | TITACCATAI | | 777777 600 |
| | | • | 640 |
| 610 | 620 | 630 | |
| | | | |
| GAGAAGGCTTCCTGC | ZACZĘACJĄTA | ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ | TTTCAA 680 |
| AGGCTACAACCTGA | ACATICCCC | TOCCAAARAAA | TIGGAA 720 |
| CGACAACGAGIICCIC | .TTTGCCCT | ACAAAAATCT(| 760 m |
| ATAGICAAAGAAGTA' | I'I'IGAGCCC | | 110110 .00 |
| AACTCGGAACTGACC | ACICCITG | AALAI IALLI. | IICCAN DOO |
| 810 | 820 | 830 . | 840 |
| لسلسلسل | سيلين | سيبليب | لسبل |
| GITCAACCICICAAA | GIIGCCII | 'I'TAAAAGCT | TTCAAC 840 |
| ATCGTTCGTGAGGTT | ITCGGGGAG | GGAGTATACC | TCGGAG 880 |
| GAGGCGGATACCATC | | | |
| CCTAATCTGGTGCGA | CTTTCGGC | AAGGGAAGIG | CCGGAA 960 |
| AAGCTAAACAATAAA | CAAAAGAC | CTTTTAAAGA | GTATAG 1000 |
| 1010 | 1020 | 1030 | 1040 |
| <u></u> | | | لببيا |
| ACTTIGAAGAGTTIG | ACGACGAC | TGGACCGCTC | GTACAT 1040 |
| GCTCGAAACCCTAAA | GGACCCCTC | GAGAGGAGGA | GAGGTA 1080 |
| AGGAAAGAAGTAAAG | GATACACTI | GAAAAGGCGA | AAGCCT 1120 |
| CATCUTA 1127 | | | , |
| eli. | emme. | SHEET (RU | F 26) |
| 3Ar | MIIIOIT | Altern /mai | mm 404/ |
| | | | |

Figure 15

| | 10 | 20 | 30 | 40 | |
|-------------------------------|-------------------------------------|-------------------------------------|------------------------|-------------------------------|------------|
| ببلبيين | لتستثلين | بصلتين | بتتليينا | بلبيسك | |
| MKKVKLI | GILDYGKY. | RYPKNHPLK | IPRVSLLLR | FLDAMNL | 4 0 |
| IDEKELI | KSRPATKE | ELLLFHIED | YINTIMEAE | RŞQSVPK | 80 |
| GAREKYN | IIGGYENPV | SYAMFTGSS | LATGSTVQA | TEEFLKG | 120 |
| NVAFNPA | AGGMHHAFK | SRANGFCYI | NDPAVGIEY | LRKKGFK | 160 |
| RILYIDI | DAHHCDGV | QEAFYDIDQ | VFVLSLHQS | PEYAFPF | 200 |
| | .210 | 220 | 230 | 240 |) |
| • | | | | | |
| سلىتت | لتتبلين | سيلب | سلسبا | لتتثلث | |
| | | | GLNDNEFLE | | 240 |
| EKGFLEE | EIGEGKGKG | YNLNIPLPK | | ALEKSLE | |
| EKGFLEE | EDEVATTÕT ETGECKCKC | YNLNIPLPK GTDPLLEDY | GLNDNEFLF | ALEKSLE AFLKAFN | 280 |
| EKGFLEE IVKEVFE IVREVFC | EBGAATGGG EBEAATTÕT EIGBGKGKG | YNLNIPLPK GIDPLLEDY GYHPYALAR | GLNDNEFLF LSKFNLSNV | ALEKSLE AFLKAFN SCREVPE | 280 320 |

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| Figure 16 |)-l |
|-----------|-----|
|-----------|-----|

| | | n • • | 11601010 | - | 7 | OCC B | O TD |
|--------|----------------|---------|---------------|--------|---------------|--------------|-------------|
| | | Residue | | Y | | OCC. B | Segment ID: |
| ATCM | 1 CB ALA | 2 | | | | 1.00 59.90 | AAAA |
| ATOM | ين C کنيک | 2 | 46.410 | | 73.628 | 1.00 52.57 | hành |
| ATOM | 3 O ALA | 2 | 45.780 | | 74.052 | 1.00 62.46 | AAAA ' |
| ATOM | 4 N ALA | 2 | 47.540 | | 75.673 | 1.00 59.52 | AAAA |
| | 5 CA ALA | 2 | 46.568 | 37.432 | 74.527 | 1.00 57.32 | AAAA |
| ATOM | 6 N LYS | 3 | 46.890 | | 72.389 | 1.00 39:61 | AAAA |
| ATOM | | 3 | 46.687 | | 71.440 | 1.00 29.58 | AAAA |
| ATOM | 7 CA LYS | | | 39.763 | 73.459 | 1.00 35.03 | AAAA |
| ATOM | 8 CE LYS | 3 | 47.855 | 40.007 | 71.102 | 1.00 55.16 | AAAA |
| ATOM | 9 CG LYS | . 3 | 49.217 | | | 1.00 65.28 | AAAA |
| ATOM | 10 CD LYS | 3 | 50.315 | 40.000 | 73.039 | 1.00 73.41 | AAAA |
| ATOM | 11 CE LYS | 3. | 51.700 | 40.163 | 73.655 | | . , |
| ATOM | 12 NZ LYS | 3 | 52.791 | 40.047 | 59.642 | 1.00 69.64 | AAAA |
| ATOM | 13 C LYS | 3 | 45.407 | 39.422 | 70.642 | 1.00 23.29 | AAAA |
| -ATOM | 14 O LYS | 3 | <u>44.984</u> | 38.282 | 73.487 | 1.00 27.41 | -AAAA |
| ATOM. | 15 N VAL | 4 | 44.814 | 40.498 | 70.138 | 1.00 25.18 | AAAA |
| | 16 CA VAL | 4 | 43.585 | 40.418 | 69.349 | 1.00 22.20 | AAAA |
| MOTA | 17 CB VAL | 4 | 42.501 | 41.365 | 59.887 | 1.00 31.46 | AAAA - |
| ATOM | - : | 4 | 41.214 | 41.202 | 59.066 | 1.00 26.55 | AAAA |
| ATOM | | 4 | 42.244 | 41.080 | 71.348 | 1.00 34.98 | AAAA |
| MOTA | 19 CG2 VAL | 4 | 43.983 | 40.851 | 67.961 | 1.00 25.33 | AAAA |
| ATOM | 20 C VAL | | 44.557 | 41.927 | 57.778 | 1.00 21.19 | AAAA |
| ATOM | 21 0 VAL | 4 | | | 56.978 | 1.00 21.32 | AAAA |
| ATOM | 22 N LYS | 5 | 43.654 | 40.023 | | 1.00 20.10 | AAAA |
| ATOM | 23 CA LYS | 5 | 44.352 | 40.291 | 55.607 | | AAAA |
| MOTA | 24 CB LYS | 5 | 45.047 | 39.214 | 55.177 | 1.00 23.35 | AAAA |
| ATOM | 25 CG LYS | 5 | 46.301 | 39.092 | 55.049 | 1.00 23.75 | |
| ATOM | 26 CD LYS | 5 | 47.183 | 40.334 | 55.919 | 1.00 23.70 | AAAA |
| ATOM | .27 CE LYS | 5 | 48.510 | 40.151 | 55.669 | 1.00 24.34 | AAAA |
| ATOM | 28 NZ LYS | 5 | 49.351 | 41.397 | £6.585 | 1.00 22.04 | AAAA |
| ATOM | 29 C LYS | 5 | 42.914 | 40.294 | £4.596 | 1.00 20.27 | AAAA |
| ATOM | 30 O LYS | 5 | 41.949 | 39.535 | 54.728 | 1.00 18.48 | AAAA |
| | 31 N LEU | 6 | 43.071 | 41.111 | 63.564 | 1.00 19.28 | AAAA |
| ATOM . | _ | 6 | 42.097 | 41.156 | 52.483 | 1.00 20.68 | AAAA |
| MOTA | | 6 | 41.571 | 42.574 | 52.291 | 1.00 23.51 | AAAA |
| MOTA | • | 6 | 40.373 | 42.712 | 51.342 | 1.00 30.59 | AAAA |
| MOTA | 34 CG LEU | 6 | 40.079 | 44.192 | 51.153 | 1.00 29.90 | AAAA |
| ATOM | 35 CD1 LEU | | 40.657 | 42.085 | 59.995 | 1.00 38.98 | AAAA |
| MOTA | 36 CD2 LEU | 6 | | 40.701 | 51.237 | 1.00 13.17 | AAAA |
| ATOM | 37 C LEU | 6 | 42.964 | 41.249 | 50.919 | 1.00 22.31 | 4666 |
| MOTA | 38 O LEU | . 6 | 43.911 | | 50.538 | 1.00 19.15 | AAAA |
| MOTA | 39 N ILE | 7 | 42.359 | 39.689 | 59.338 | 1.00 13.38 | AAAA |
| ATOM | 40 CA ILE | 7 | 43.045 | 39.199 | | 1.00 19.05 | AAAA : |
| ATOM | 41 CE ILE | 7 | 42.922 | 37.674 | 59.191 | | AAAA |
| ATOM | 42 CG2 TLE | 7 | 43.930 | 37.162 | 53.144 | | AAAA |
| ATOM | ;3 CG1 ILE | 7 | 43.253 | 37.007 | 60.521 | | AAAA |
| ATOM | 44 CD1 ILE | 7 | 43.296 | 35.543 | 50.450 | | |
| ATOM | 45 C ILE | 7 | 42.396 | 39.850 | 58.125 | | AAAA . |
| ATOM | 46 0 ILE | 7 | 41.188 | 39.729 | 57.928 | | áááá |
| ATOM | 47 N GLY | 8 | 43.193 | 40.562 | | | AAAA. |
| ATOM | 48 · CA GLY | 9 | 42.523 | 41.193 | 55.148 | 1.00 13.11 | AAAA |
| | 49 C GLY | 8 | 43.640 | 41.857 | 55.243 | 1.00 20.91 | AAAA |
| ATOM | ' | | 44.849 | | 55.504 | | AAAA |
| ATOM | JO 0 | 9 | 43.134 | | | 1.00 23.99 | AAAA 🗎 |
| ATOM | | ğ | 43.950 | | | | AAAA |
| ATOM | 52 CA THR | | 44.739 | | | | AAAA ' |
| ATOM | 53 CE THR | 9 | 45.321 | | | | AAAA |
| ATOM | 54 CG1 THR | 9 | | | | | AAAA |
| MOTA | 55 CG2 THR | 9 | 43.823 | | | 1.00 29.04 | |
| ATOM | 56 C THR | 9 | 43.025 | | | | AAAA |
| ATOM | 57 O THR | | 41.572 | | | | |
| ATOM | 58 N LEU | 10 | 43.517 | | | | AAAA |
| ATCM | 59 CA LEU | 10 | 42.690 | | | | |
| ATCM | 60 CB LEU | | 43.256 | | | 1.00 28.09 | |
| ATOM | 51 CG LEU | | 43.142 | 48.266 | | | AAAA |
| | 62 CD1 LEU | | 41.680 | 48.403 | | | AAAA |
| ATOM | 63 CD2 LEU | | 43.938 | 47.744 | : 53.126 | 1.00 41.33 | AAAA |
| ATCM | | | 42.556 | | 49.512 | 1.00 32.68 | AAAA |
| ATOM | | | 41.73 | | . ≟8.70 | 2 1.00 26.97 | AAAA |
| ATCM | | | 43.37 | | | 6 1.00 25.75 | i aaaa |
| ATCM | 56 N ASP | | | | | | |

Figure 16-2

| MOTA | 67 CA ASP | | 43.36 | 7 43.54 | 1 47.970 | 1.00 35.74 | |
|--------------|-------------------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 68 CB ASP | | 44.47 | 7 42.48 | | | AAAA AAAA |
| MOTA | 69 CG ASP | | 45.85 | 8 43.09 | | | AAAA |
| MOTA | 70 OD1 ASP | 11 | 46.11 | | | | AAAA |
| MOTA MOTA | 71 OD2 ASP 72 C ASP | 11 | 46.69 | | | | AAAA |
| ATOM | | 11 | 42.034 | | | 1.00 34.26 | AAAA |
| ATOM | | 11 | 41.748 | | | 1.00 31.12 | AAAA |
| ATOM | 74 N TYR 75 CA TYR | 12 | 41.220 | 42.55 | | | AAAA |
| ATOM | 76 CB TYR | 12 12 | 39.923 | | | | AAAA |
| ATOM | 77 CG TYR | 12 | 39.119 39.648 | 41.72 | | | AAAA |
| ATOM | 78 CD1 TYR | 12 | 40.137 | | | | AAAA |
| MOTA | 79 CE1 TYR | 12 | 40.592 | | | | AAAA |
| MOTA | 80 CD2 TYR | 12 | 39.629 | | | 1.00.30.35 | AAAA |
| ATOM | 81 CE2 TYR | 12 | 40.077 | | | 1.00 22.97 1.00 19.60 | AAAA |
| ATOM | 82 CZ TYR | 12 | 40.554 | | | 1.00 19.60 | AAAA |
| MOTA | 83 OH TYR | 12 | 40.964 | 37.456 | | 1.00 23.49 | AAAA |
| ATOM | 84 C TYR | 12 | 39.144 | 42.907 | 47.390 | 1.00 26.67 | AAAA AAAA |
| ATOM | 85 O TYR | 12 | 38.307 | 42.466 | 46.593 | 1.00 30.51 | AAAA |
| ATOM ATOM | 86 N GLY | 13 | 39.441 | 44.201 | 47.492 | 1.00 30.22 | AAAA |
| ATOM | 87 CA GLY 88 C GLY | 13 | . 38.767 | | | 1.00 25.13 | AAAA |
| ATOM | 88 C GLY | 13 | 38.911 | 45.009 | | 1.00 27.31 | AAAA |
| ATOM | 90 N LYS | 13 14 | 38.096 | 45.522 | | 1.00 29.38 | AAAA |
| ATOM | 91 CA LYS | 14 | 39.937 40.176 | 44.269 | | 1.00 33.56 | AAAA |
| ATOM | 92 CB LYS | 14 | 41.680 | 44.005 44.026 | | 1.00 39.81 | AAAA |
| MOTA | 93 CG LYS | 14 | 42:292 | | | 1.00 51.10 1.00 64.99 | AAAA |
| MOTA | 94 CD LYS | 14 | 41.757 | 46.218 | | 1.00 84.99 | AAAA |
| MOTA | 95 CE LYS | 14 | 42.183 | 45.639 | | 1.00 67.25 | AAAA |
| MOTA | 96 NZ LYS | 14 | 41.637 | 44.280 | 40.045 | 1.00 70.06 | AAAA AAAA |
| MOTA | 97 C LYS | 14 | 39.589 | 42.688 | 42.834 | 1.00 39.98 | AAAA |
| MOTA MOTA | 98 O LYS 99 N TYR | 14 | 39.746 | 42.350 | 41.658 | 1.00 46.99 | AAAA |
| MOTA | 99 N TYR 100 CA TYR | 15 | 38.927 | 41.944 | 43.717 | 1.00 32.64 | AAAA |
| ATOM | 101 CB TYR | 15 15 | 38.318 | 40.655 | 43.355 | 1.00 41.01 | AAAA |
| ATOM | 102 CG TYR | 15 | 38.996 40.496 | 39.512 39.571 | 44.126 | 1.00 26.48 | AAAA |
| ATOM | 103 CD1 TYR | 15 | 41.289 | 39.401 | 44.033 | 1.00 34.97 | AAAA |
| MOTA | 104 CE1 TYR | 15 | 42.677 | 39.548 | 45.167 45.106 | 1.00 43.28 1.00 36.05 | AAAA |
| MOTA | 105 CD2 TYR | 15 | 41.127 | 39.879 | 42.827 | 1.00 40.78 | AAAA |
| ATOM | 106 CE2 TYR | 15 | 42.508 | 40.027 | 42.756 | 1.00 37.13 | AAAA AAAA |
| ATOM | 107 CZ TYR | 15 | 43.275 | 39.865 | 43.899 | 1.00 36.87 | AAAA |
| ATOM ATOM | 108 OH TYR | 15 | 44.644 | 40.044 | 43.844 | 1.00 35.40 | AAAA |
| ATOM | 109 C TYR 110 O TYR | 15 | 36.838 | 40.705 | 43.714 | 1.00 38.62 | AAAA |
| ATOM | 110 O TYR 111 N ARG | 15 16 | 36.344 | 39.868 | 44.468 | 1.00 37.82 | AAAA |
| ATOM | 112 CA ARG | 16 | 36.141 34.716 | 41.703 | 43.177 | 1.00 44.85 | AAAA |
| ATOM | 113 CB ARG | 16 | 34.320 | 41.890 43.348 | 43.431 | 1.00 45.75 | AAAA |
| ATOM | 114 CG ARG | 16 | 35.170 | 44.399 | 43.187 43.875 | 1.00 54.17 | AAAA |
| MOTA | 115 CD ARG | 16 | 34.920 | 44.506 | 45.369 | 1.00 66.77 1.00 72.39 | AAAA |
| MOTA | 116 NE ARG | 16 | 35.649 | 45.646 | 45.923 | 1.00 72.39 | AAAA |
| MOTA | 117 CZ ARG | 16 | 35.489 | | 45.518 | 1.00 81.94 | AAAA |
| ATOM | 118 NH1 ARG | 16 | 34.624 | 47.197 | | 1.00 80.19 | AAAA AAAA |
| ATOM | 119 NH2 ARG | 16 | 36.205 | 47.878 | 46.069 | 1.00 85.46 | AAAA |
| ATOM | 120 C ARG | 16 | 33.915 | 41.029 | 42.460 | 1.00 43.50 | AAAA |
| MOTA MOTA | 121 O ARG 122 N TYR | 16 | 34.400 | 40.667 | 41.385 | 1.00 38.62 | AAAA |
| ATOM | 122 N TYR 123 CA TYR | 17 17 | 32.689 | 40.692 | | 1.00 32.68 | AAAA |
| ATOM | 124 CB TYR | 17 | 31.850 30.662 | 39.923 | | 1.00 37.55 | AAAA |
| ATOM | 125 CG TYR | 17 | 31.040 | 39.306 | | 1.00 41.05 | AAAA |
| MOTA | 126 CD1 TYR | 17 | 32.039 | 38.104 38.194 | | 1.00 37.51 | AAAA |
| MOTA | 127 CE1 TYR | 17 | 32.383 | 38.194 37.095 | | 1.00 32.59 | AAAA |
| MOTA | 128 CD2 TYR | 17 | | 36.875 | | 1.00 29.32 1.00 31.46 | AAAA |
| MOTA | 129 CE2 TYR | 17 | | 35.772 | 44.122 | 1.00 31.46 | AAAA |
| MOTA | 130 CZ TYR | 17 | | 35.887 | | 1.00 28.84 | AAAA AAAA |
| MOTA | 131 OH TYR | 17 | | 34.807 | | 1.00 27.14 | AAAA |
| MOTA | 132 C TYR | 17 | | 40.871 | | 1.00 40.97 | AAAA |
| • | • | | | | - | | |

| | | | | | | 40 007 | 40.984 | 1.00 29.58 | AAAA |
|------|-----|-----|-----|----------|------------------|---------|---------|------------|------|
| ATCM | 133 | 0 | TYR | 17 | 31.435 | 42.097 | 39.722 | 1.00 41.02 | AAAA |
| ATOM | 134 | N | PRO | 18 | 30.904 | 40.321 | | 1.00 41.02 | AAAA |
| MOTA | 135 | CD | PRO | 18 | 30.760 | 38.910 | 39.318 | 1.00 49.35 | AAAA |
| ATCM | 136 | CA | PRO | 18 | 30.459 | 41.197 | 38.649 | | AAAA |
| ATCM | 137 | CB | PRO | 18 | 30.321 | 40.228 | 37.481 | 1.00 59.04 | |
| ATCM | 138 | CG | PRO | 18 | 29.756 | 39.017 | 38.179 | 1.00 54.15 | AAAA |
| ATOM | 139 | С | PRO | 18 | 29.178 | 41.982 | 38.864 | 1.00 54.97 | AAAA |
| ATOM | 140 | Ō | PRO | 18 | 28.457 | 41.823 | 39.850 | 1.00 46.85 | AAAA |
| ATOM | 141 | N | LYS | 19 | 28.961 | 42.868 | 37.904 | 1.00 60.87 | AAAA |
| | 142 | CA | LYS | 19 | 27.777 | 43.696 | 37.749 | 1.00 67.78 | AAAA |
| ATOM | 143 | CB | LYS | 19 - | 27.155 | 43.278 | 36.425 | 1.00 73.26 | AAAA |
| ATOM | 144 | CG | LYS | 19 | 26.971 | 41.752 | 36.414 | 1.00 77.87 | AAAA |
| ATOM | 145 | CD | LYS | 19 | 26.276 | 41.166 | 35.209 | 1.00 81.01 | AAAA |
| ATOM | 146 | CE | LYS | 19 | 26.039 | 39.680 | 35.471 | 1.00 82.45 | AAAA |
| ATOM | 147 | NZ | LYS | 19 | 25.417 | 38.959 | 34.331 | 1.00 83.11 | AAAA |
| MOTA | 148 | C | LYS | 19 | 26.688 | 43.594 | 38.814- | 1.00 64.15 | AAAA |
| MOTA | 149 | Ö | LYS | 19 | 26.810 | 44.047 | 39.949 | 1.00 65.73 | AAAA |
| ATOM | | N | ASN | | 25.604 | 42.986 | 38.345 | 1.00 59.78 | AAAA |
| ATOM | 150 | CA | ASN | 20 | 24.353 | 42.703 | 39.025 | 1.00 59.91 | AAAA |
| MOTA | 151 | | ASN | 20 | 23.516 | 41.844 | 38.077 | 1.00 68.08 | AAAA |
| ATOM | 152 | CB | ASN | 20 | 22.108 | 42.355 | 37.907 | 1.00 78.73 | AAAA |
| MOTA | 153 | CG | | 20 | 21.894 | 43.498 | 37.496 | 1.00 78.67 | AAAA |
| MOTA | 154 | OD1 | | 20 | 21.132 | 41.505 | 38.211 | 1.00 83.22 | AAAA |
| MOTA | 155 | | ASN | | 24.474 | 41.977 | 40.361 | 1.00 53.35 | AAAA |
| MOTA | 156 | C | ASN | 20 20 | 23.611 | 42.112 | 41.234 | 1.00 59.92 | AAAA |
| MOTA | 157 | 0 | ASN | | 25.543 | 41.206 | 40.511 | 1.00 44.23 | AAAA |
| ATOM | 158 | N | HIS | 21 · | 25.768 | 40.397 | 41.7.07 | 1.00 28.15 | AAAA |
| ATCM | 159 | CA | HIS | 21 | 27.088 | 39.639 | 41.570 | 1.00 31.84 | AAAA |
| MOTA | 160 | CB | HIS | 21 | 27.155 | 38.411 | 42.418 | 1.00 34.79 | AAAA |
| MOTA | 161 | CG | HIS | 21 | 27.133 | 38.259 | 43.752 | 1.00 25.03 | AAAA |
| ATOM | 162 | | HIS | 21 | 26.929 | 37.148 | 41.917 | 1.00 34.81 | AAAA |
| MOTA | 163 | | HIS | 21 | 26.979 | 36.269 | 42.900 | 1.00 17.01 | AAAA |
| ATOM | 164 | | HIS | 21 | 27.228 | 36.917 | 44.026 | 1.00 32.31 | AAAA |
| MOTA | 165 | | HIS | 21 | 27.220 | -41.135 | 43.051 | 1.00 29.37 | AAAA |
| ATOM | 166 | С | HIS | 21 | 26.346 | 42.210 | 43.186 | 1.00 28.54 | AAAA |
| ATOM | 167 | 0 | HIS | 21 | 25.093 | 40.565 | 44.066 | 1.00 29.14 | AAAA |
| ATOM | 168 | N | PRO | 22 | 24.301 | 39.322 | 44.061 | 1.00 31.20 | AAAA |
| ATOM | 169 | CD | PRO | 22 | 25.034 | 41.185 | 45.395 | 1.00 32.84 | AAAA |
| ATOM | 170 | CA | PRO | 22 | 24.174 | 40.192 | 46.187 | 1.00 34.98 | AAAA |
| MOTA | 171 | CB | PRO | 22 | 23.257 | 39.634 | 45.109 | 1.00 30.11 | AAAA |
| ATOM | 172 | CG | PRO | 22 | 26.411 | 41.415 | 46.044 | 1.00 34.37 | AAAA |
| atom | 173 | C | PRO | 22 | 26.554 | 42.272 | 46.916 | 1.00 29.17 | AAAA |
| atom | 174 | 0 | PRO | 22 | 27.415 | 40.644 | 45.629 | 1.00 29.22 | AAAA |
| ATOM | 175 | N | LEU | 23 | 28.765 | 40.781 | 46.181 | 1.00 26.49 | AAAA |
| ATOM | 176 | CA | LEU | 23 | 29.414 | 39.397 | 46.332 | 1.00 22.30 | AAAA |
| ATOM | 177 | CB | LEU | 23 | 28.703 | 38.527 | 47.380 | 1.00 21.04 | AAAA |
| ATOM | 178 | CG | LEU | 23 | 29.307 | 37.113 | 47.410 | 1.00 19.35 | AAAA |
| ATOM | 179 | | LEU | 23 | _ | 39.197 | 48.746 | 1.00 26.51 | AAAA |
| ATOM | 180 | | LEU | 23 | 28.850 29.661 | 41.718 | 45.361 | 1.00 25.81 | AAAA |
| ATOM | 181 | С | LEU | 23 | | 41.693 | 45.477 | 1.00 28.45 | AAAA |
| ATOM | 182 | 0 | LEU | 23 | 30.893 | 42.539 | 44.532 | 1.00 24.86 | AAAA |
| ATOM | 183 | N | LYS | 24 | 29.018 | 43.552 | 43.723 | 1.00 27.35 | AAAA |
| ATOM | 184 | CA | LYS | 24 | 29.696 | 44.244 | 42.830 | 1.00 28.57 | AAAA |
| ATOM | 185 | CB | LYS | 24 | 28.662 | 45.532 | 42.171 | 1.00 52.95 | AAAA |
| ATOM | 186 | CG | LYS | 24 | 29.118 | 46.603 | 42.283 | 1.00 63.74 | AAAA |
| MOTA | 187 | CD | LYS | 24 | 28.025 | 46.138 | 41.706 | 1.00 66.09 | AAAA |
| ATOM | 188 | CE | LYS | 24 | 26.688 | | 41.896 | 1.00 66.00 | AAAA |
| ATOM | 189 | NZ | LYS | 24 | 25.595 | 47.137 | 44.676 | 1.00 29.52 | AAAA |
| ATOM | 190 | С | LYS | 24 | 30.332 | 44.592 | 44.420 | | AAAA |
| ATOM | 191 | 0 | LYS | 24 | 31.412 | 45.123 | 45.779 | | AAAA |
| ATOM | 192 | N | ILE | 25 | 29.652 | 44.879 | 46.738 | | AAAA |
| ATOM | 193 | CA | ILE | 25 | 30.151 | 45.865 | 47.824 | | AAAA |
| ATOM | 194 | CB | ILE | 25 | 29.105 | 46.177 | | | AAAA |
| ATOM | 195 | CG2 | ILE | 25 | 27.961 | 46.951 | | | AAAA |
| ATOM | 196 | CG1 | ILE | 25 | 28.661 | 44.869 | 40 | | AAAA |
| ATOM | 197 | CD1 | ILE | 25 | 27.718 | 45.051 | 40 400 | | AAAA |
| ATOM | 198 | С | ΪLΕ | 25 | 31.424 | 45.463 | 47.483 | 1.00 36.13 | |
| | | | • | | | | | | |

| MOTA | 199 | 9 0 | ILE | 25 | 31.73 | 6 44.271 | 47.623 | 1.00 26.54 | AAAA I |
|--------------|-------------|----------|------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 200 | | PRO | 26 | 32.19 | | 47.956 | | AAAA |
| MOTA | 201 | | PRO | 26 | 31.97 | | | | |
| ATOM | 202 203 | | PRO PRO | 26 | 33.43 | | 48.707 | | |
| MOTA - | 203 | | PRO | 26 26 | 34.016 33.39 | | 48.814 47.617 | 1.00 34.29 | |
| MOTA | 205 | | PRO | 26 | 32.94 | | 50.061 | 1.00 43.39 | |
| ATOM | 206 | | PRO | 26 | 31.85 | | 50.484 | 1.00 25.51 | |
| | 207 | | ARG | 27 | 33.719 | | 50.743 | 1.00 21.98 | |
| ATOM | 208 | CA | ARG | 27 | 33.26 | • | 52.035 | 1.00 26.17 | |
| MOTA | 209 | • | ARG | 27 | 32.643 | L 42.969 | 51.834 | 1.00 22.70 | |
| ATOM | 210 | | ARG | . 27 | 31.442 | | 50.890 | 1.00 26.75 | |
| ATÓM | 211 | | ARG | 27 | 30.832 | | 50.581 | | |
| ATOM ATOM | 212 213 | | ARG ARG | 27 27 | 30.121 30.582 | | 51.716 | 1.00 28.66 | |
| MOTA | 213 | | | 27 | 31.778 | | 52.503 52.290 | 1.00 31.79 | |
| ATOM | 215 | | ARG | 27 | 29.833 | | 53.505 | 1.00 26.16 | |
| MOTA | 216 | | ARG | 27 | 34.358 | | 53.090 | 1.00 24.10 | |
| MOTA | 217 | 0 | ARG | 27 | 34.326 | | 54.038 | 1.00 23.50 | |
| MOTA | 218 | | VAL | - 28 | 35.314 | 43.390 | 52.960 | 1.00 21.45 | |
| MOTA | 219 | | VAL | 28 | 36.385 | | 53.953 | 1.00 21.75 | |
| MOTA | 220 | | VAL | 28 | 37.221 | | 53.866 | 1.00 26.55 | |
| MOTA MOTA | 221 222 | | VAL VAL | 28 28 | 38.407 | | 54.830 | 1.00 23.84 | |
| MOTA | 223 | C | VAL | 28 | 36.337 37.277 | | 54.214 53.736 | 1.00 19.20 | |
| ATOM | 224 | ō | VAL | 28 | 37.770 | | 54.702 | 1.00 25.15 | |
| ATOM | 225 | N · · | - | 29 | 37.480 | | 52:475 | 1.00 19.22 | |
| MOTA | 226 | CA | SER | . 29 | 38.320 | 46.169 | 52.209 | 1.00 19.63 | |
| MOTA | 227 | CB | SER | 29 | 38.591 | | 50.702 | 1.00 24.45 | |
| MOTA | 228 | oG | SER | 29 | . 37.411 | | 49.984 | 1.00 28.74 | |
| ATOM ATOM | 229 230 | С 0 | SER SER | 29 29 | 37.579 38.184 | | 52.756 | 1.00 21.50 | |
| ATOM | 231 | N | LEU | 30 | 36.256 | | 53.271 52.673 | 1.00 18.95 1.00 19.56 | |
| ATOM | 232 | CA | LEU | 30 | 35.499 | | 53.177 | 1.00 25.97 | |
| ATOM | 233 | CB | LEU | 30 | 34.032 | | 52.744 | 1.00 22.90 | |
| ATOM | 234 | CG | LEU | 30 | 33.085 | | 53.157 | 1.00 26.62 | AAAA |
| MOTA | 235 | | LEU | 30 | 32.885 | | 54.648 | 1.00 38.27 | |
| ATOM | 236 | CD2 | LEU | 30 30 | 33.653 | | 52.698 | 1.00 25.71 | |
| ATOM ATOM | 237 | 0 | LEU | 30 | 35.604 35.704 | 48.509 49.580 | 54.696 55.273 | 1.00 18.44 1.00 25.05 | |
| ATOM | 239 | N | LEU | 31 | 35.578 | 47.336 | 55.336 | 1.00 25.05 | |
| ATOM | 240 | CA | LEU | 31 | 35.672 | 47.270 | 56.797 | 1.00 20.47 | |
| ATOM | 241 | CB | LEU | 31 | 35.613 | 45.821 | 57.300 | 1.00 20.60 | |
| MOTA | 242 | CG | LEU | 31 | 34.988 | 45.456 | 58.665 | 1.00 39.80 | |
| MOTA | 243 | CD1 | | 31 | 35.712 | 44.219 | 59.257 | 1.00 23.99 | |
| MOTA | 244 245 | CD2 C | LEU | 31 31 | 35.085 | 46.591 | 59.637 | 1.00 28.48 | |
| ATOM ATOM | 246 | ò | LEU | 31 | 37.009 37.070 | 47.870 48.673 | 57.229 58.154 | 1.00 23.85 1.00 21.24 | |
| ATOM | 247 | N | LEU | 32 | 38.079 | 47.462 | 56.562 | 1.00 23.91 | |
| ATOM | 248 | | LEU | 32 | 39.400 | 47.965 | 56.899 | 1.00 24.82 | |
| MOTA | 249 | | LEU | 32 | 40.479 | 47.320 | 56.018 | 1.00 24.81 | |
| MOTA | 250 | CG | LEU | 32 | 40.849 | 45.854 | 56.276 | 1.00 27.00 | AAAA |
| ATOM | 251 | CD1 | | 32 | 41.995 | 45.435 | 55.354 | 1.00 27.13 | AAAA |
| MOTA | . 252 | CD2 | | 32 | 41.285 | 45.687 | 57.720 | 1.00 34.49 | AAAA |
| MOTA | 253 254 | | LEU LEU | 32 32 | 39.466 39.958 | 49.475 | 56:763 57.662 | 1.00 19.56 1.00 20.71 | AAAA |
| ATOM ATOM | 255 | | ARG | 33 | 38.974 | 50.143 50.006 | 55.645 | 1.00 23.25 | AAAA AAAA |
| ATOM | 256 | | ARG | 33 | 39.007 | 51.449 | 55.441 | 1.00 24.33 | AAAA |
| ATOM | 257 | | ARG | 33 | 38.575 | 51.806 | 54.013 | 1.00 23.46 | AAAA |
| MOTA | 258 | | ARG | 33 | 39.571 | 51.327 | 52.945 | 1.00 26.94 | AAAA |
| MOTA | 259 | | ARG | 33 | 39.337 | 51.976 | 51.585 | 1.00 42.13 | AAAA |
| MOTA | 360 | | ARG | 33 | 38.023 | 51.661 | 51.037 | 1.00 59.06 | , AAAA |
| MOTA | 261 | | ARG | 33 | 37.583 | 52.088 | 49.857 | 1.00 60.87 | AAAA |
| MOTA | 262 | NH1 | | 33 33 | 38.353 | 52.850 | 49.095 | 1.00 65.33 | AAAA |
| MOTA MOTA | ·263 264 | NH2 | | 33 33 | 36.373 38.124 | 51.743 | 49.433 56.455 | 1.00 56.24 1.00 30.33 | AAAA |
| 21 OII | ~ 04 | - 1 | ARG | | JU.124 | 52.156 | JU.4JJ | ±.00 J0.JJ | AAAA |

| | | | | | | | 55 005 | 1.00 25.45 | AAAA |
|------|------|-----|------|-------|-----------------|----------|--------|------------|--------|
| ATOM | 265 | 0 | ARG | 33 | 38.441 | 53.252 | 56.905 | 1.00 23.93 | |
| ATOM | 266 | N | PHE | 34 | 37.022 | 51.514 | 56.828 | 1.00 24.98 | AAAA |
| | 267 | CA | PHE | 34 | 36.099 | 52.085 | 57.789 | 1.00 27.09 | AAAA |
| MOTA | 268 | CB | PHE | 34 | 34.798 | 51.276 | 57.807 | 1.00 24.88 | AAAA |
| ATOM | | | PHE | 34 | 33.719 | 51.898 | 58.631 | 1.00 20.46 | AAAA |
| MOTA | 269 | CG | | | 33.043 | 53.018 | 58.171 | 1.00 18.74 | AAAA |
| MOTA | 270 | | PHE | 34 | | 51.383 | 59.889 | 1.00 20.19 | AAAA |
| MOTA | 271 | CD2 | PHE | 34 | 33.396 | | | 1.00 23.04 | AAAA |
| ATOM | 272 | CE1 | PHE | 34 | 32.043 | 53.627 | 58.956 | 1.00 25.08 | AAAA |
| ATOM | 273 | CE2 | PHE | . 34. | 32.406 | 51.974 | 60.681 | | |
| ATOM | 274 | CZ | PHE | 34 | 31.726 | 53.104 | 60.209 | 1.00 23.31 | AAAA |
| | 275 | c | PHE | 34 | 36.709 | 52.115 | 59.194 | 1.00 23.93 | AAAA |
| MOTA | | Ö | PHE | 34 | 36.668 | 53.138 - | 59.883 | 1:00 21.71 | ``AAAA |
| MOTA | 276 | | | 35 | 37.298 | 51.013 | 59.645 | 1.00 21.33 | AAAA . |
| ATOM | 277 | N | LYS | | 37.862 | 51.084 | 60.978 | 1.00 22.54 | AAAA |
| MOTA | 278 | CA | LYS | 35 | | 49.716 | 61.476 | 1.00 29.70 | AAAA |
| ATOM | 279 | CB | LYS | 35 | 38.276 | | 61.924 | 1.00 29.48 | AAAA |
| ATOM | 280 | CG | LYS | 35 | 37.082 | 48.890 | | 1.00 42.17 | AAAA |
| MOTA | 281 | CD | LYS | 35 | 37.517 | 47.535 | 62.398 | | AAAA |
| ATOM | 282 | CE | LYS | 35 | 38.157 | 46.762 | 61.275 | 1.00 34.89 | |
| ATOM | 283 | NZ | LYS | 35 | 39.372 | 47.412 | 60.719 | 1.00 67.18 | AAAA |
| - | 284 | C | LYS | 35 | 39.027 | 52.055 | 61.040 | 1.00 24.68 | AAAA |
| MOTA | | Ö | LYS | 35 | 39.282 | 52.640 | 62.085 | 1.00 22.33 | AAAA |
| ATOM | 285 | | | 36 | 39.724 | 52.231 | 59.926 | 1.00 25.67 | AAAA |
| MOTA | 286 | N | ASP | | 40.842 | 53.163 | 59.898 | 1.00 25.57 | AAAA |
| ATOM | 287 | CA | ASP | 36 | | 52.984 | 58.621 | 1.00 32.26 | AAAA |
| MOTA | 288 | CB | ASP | 36 | 41.669 | 53.914 | 58.572 | 1.00 33.92 | AAAA |
| ATOM | 289 | CG | ASP | 36 | 42.881 | | | 1.00 40.22 | AAAA |
| ATOM | 290 | OD1 | ASP | 36 | 43.641 | 53.969 | 59.563 | 1.00 40.22 | AAAA |
| ATOM | 291 | OD2 | ASP | 36 | 43.078 | 54.575 | 57.538 | | AAAA |
| MOTA | 292 | С | ASP | 36 | 40.285 | 54.578 | 59.973 | 1.00 28.04 | |
| | 293 | ō | ASP | 36 | 40.761 | 55.397 | 60.765 | 1.00 29.52 | AAAA |
| ATOM | | N | ALA | 37 | 39.272 | 54.864 | 59.159 | 1.00 23.32 | AAAA |
| ATOM | 294. | | ALA | 37 | 38.651 | 56.192 | 59.163 | 1.00 28.22 | AAAA |
| MOTA | 295 | CA | | 37 | 37.506 | 56.251 | 58.119 | 1.00 25.93 | AAAA |
| ATOM | 296 | CB | ALA | | 38.127 | 56.549 | 60.565 | 1.00 28.41 | AAAA |
| ATOM | 297 | C | ALA | 37 | | 57.708 | 60.972 | 1.00 29.27 | AAAA |
| ATOM | 298 | 0 | ALA | 37 | 38.186 | | 61.300 | 1.00 24.76 | AAAA |
| ATOM | 299 | N | MET. | 38 | 37.639 | 55.547 | 62.669 | 1.00 25.45 | AAAA |
| ATOM | 300 | CA | MET | 38 | 37.103 | 55.727 | | 1.00 25.45 | AAAA |
| ATOM | 301 | CB | MET | 38 | 36.077 | 54.625 | 62.982 | | AAAA |
| MOTA | 302 | CG | MET | 38 | 34.816 | 54.660 | 62.148 | | AAAA |
| | 303 | SD | MET | 38 | 33.733 | 55.983 | 62.702 | 1.00 29.90 | |
| MOTA | 304 | CE | MET | 38 | 33.402 | 55.417 | 64.376 | 1.00 26.51 | AAAA |
| ATOM | 305 | c | MET | 38 | 38.203 | 55.667 | 63.744 | 1.00 26.42 | AAAA |
| ATOM | | o | MET | 38 | 37.924 | 55.818 | 64.947 | 1.00 23.77 | AAAA |
| MOTA | 306 | | | 39 | 39.437 | 55.434 | 63.300 | 1.00 26.21 | AAAA |
| ATOM | 307 | N | ASN | | 40.607 | 55.308 | 64.170 | 1.00 28.53 | AAAA |
| ATOM | 308 | CA | ASN | 39 | | 56.643 | 64.855 | 1.00 33.95 | AAAA |
| ATOM | 309 | CB | ASN | 39 | 40.926 | | 63.858 | 1.00 29.46 | AAAA |
| ATOM | 310 | CG | ASN | 39 | 41.153 | 57.751 | 62.925 | 1.00 36.28 | AAAA |
| ATOM | 311 | OD1 | ASN | 39 | 41.930 | 57.596 | | 1.00 40.03 | AAAA |
| ATOM | 312 | ND2 | ASN | 39 | 40.472 | 58.880 | 64.046 | | AAAA |
| ATOM | 313 | С | ASN | 39 | 40.374 | 54.223 | 65.205 | 1.00 30.07 | |
| | 314 | 0 | ASN | 39 | 40.682 | 54.390 | 66.395 | 1.00 25.47 | AAAA |
| ATOM | 315 | N | LEU | 40 | 39.814 | 53.105 | 54.744 | 1.00 28.19 | AAAA |
| ATOM | | | | 40 | 39.527 | 51.984 | 65.633 | 1.00 25.50 | AAAA |
| MOTA | 316 | CA | LEU | | 38.060 | 51.562 | 65.514 | 1.00 32.14 | AAAA |
| MOTA | 317 | CB | LEU | 40 | 37.044 | 52.585 | 66.036 | 1.00 30.47 | AAAA |
| MOTA | 318 | CG | LEU | 40 | | | 65.894 | 1.00 29.07 | AAAA · |
| MOTA | 319 | CD1 | LEU | 40 | 35.637 | 52.027 | 67.491 | 1.00 23.80 | AAAA |
| ATOM | 320 | CD2 | LEU | 40 | 3 7 .325 | 52.889 | | 1.00 26.99 | AAAA |
| ATOM | 321 | С | LEU | 40 | 40.433 | 50.771 | 65.415 | 1.00 25.41 | AAAA |
| MOTA | 322 | 0 | LEU | 40 | 40.157 | 49.683 | 65.915 | 1.00 23.41 | AAAA |
| | 323 | N | ILE | 41 | 41.528 | 50.970 | 64.691 | 1.00 28.33 | |
| MOTA | 324 | CA | ILE | 41 | 42.459 | 49.882 | 64.459 | 1.00 25.08 | AAAA |
| ATOM | | | ILE | 41 | 42.010 | 49.020 | 63.243 | 1.00 25.01 | AAAA |
| ATCM | 325 | CB | | 41 | 42.061 | 49.824 | 61.961 | 1.00 22.74 | AAAA |
| MOTA | 326 | | ILE | | 42.917 | 47.802 | 63.128 | 1.00 31.01 | AAAA |
| MOTA | 327 | | ILE | 41 | | | 64.341 | 1.00 42.18 | AAAA |
| ATCM | 328 | | ILE | 41 | 42.895 | 46.951 | C4 047 | 1.00 24.09 | AAAA |
| ATOM | 329 | С | ILE | 41 | 43.900 | 50.376 | | 1.00 28.92 | AAAA |
| ATOM | 330 | 0 | ILE | 41 | 44.128 | 51.406 | 021 | 1.00 20.74 | • |
| | | • | | | | • | | | |

| MOTA | 331 N ASP | 42 | 44.86 | 6 49.63 | 4 64.787 | 7 1 00 00 00 | |
|--------|-------------|------|----------|---------|----------|--------------|--------|
| ATOM | | | • | | | | AAAA |
| | | | 46.27 | | 8 64.638 | 3 1.00 32.52 | AAAA |
| MOTA | 333 CB ASP | | 46.95 | 1 50.09 | 4 66.007 | | 3333 |
| ATOM | 334 CG ASP | 42 | 46.26 | | | 1.00 54.24 | AAAA |
| MOTA | 335 OD1 ASP | | | | | | AAAA |
| | | | 46.079 | 9 52.25 | 0 66.467 | 1.00 50.19 | AAAA |
| MOTA | 336 OD2 ASP | 42 | 45.924 | 4 50.73 | 6 68.062 | | |
| ATOM | 337 C ASP | 42 | 46.985 | | | 1.00 33.00 | AAAA |
| MOTA | | | | | | | . AAAA |
| | | | 46.594 | 47.75 | 8 63.838 | 1.00 26.71 | AAAA |
| ATOM | 339 N GLU | 43 | 48.036 | 49.31 | 2 63.092 | | |
| MOTA | 340 CA GLU | 43 | 48.793 | | | 1.00 29.99 | AAAA |
| ATOM | | _ | | | | | AAAA |
| | | 43 | 50.078 | 3 49.04 | 5 61.724 | 1.00 36.12 | AAAA |
| MOTA | 342 CG GLU | 43 | 49.886 | 50.118 | | | |
| MOTA | 343 CD GLU | 43 | 51.214 | | | 1.00 52.72 | AAAA |
| . ATOM | | | | | | | AAAA |
| | | 43 | 51.928 | 49.688 | 3 59.536 | 1.00 70.32 | AAAA |
| ATOM | 345 OE2 GLU | 43 | 51.550 | 51.755 | | 1.00 60.38 | |
| ATOM | 346 C GLU | 43 | 49.196 | | | | AAAA |
| MOTA | | • | | | | | AAAA |
| | | 43 | 49.125 | 46.024 | 62.209 | 1.00 36.83 | AAAA |
| ATOM | 348 N LYS | 44 | 49.636 | 47.103 | | | |
| ATOM | 349 CA LYS | 44 | 50.084 | | | 1.00 20.20 | AAAA |
| MOTA | | | | | | | AAAA |
| | | 44 | 50.974 | 46.245 | 65.927 | 1.00 44.28 | AAAA |
| MOTA | 351 CG LYS | 44 | 52.211 | 47.007 | | | |
| ATOM | 352 CD LYS | 44 | 53.187 | | | | AAAA |
| ATOM | | | . 33.107 | 47.449 | | , | AAAA |
| | | 44 | 54.373 | 48.167 | 65.849 | 1.00 67.21 | AAAA |
| ATOM | 354 NZ LYS | 44 | 55.361 | 48.648 | 66.850 | | |
| ATOM | 355 C LYS | 44 | 48.982 | | | | AAAA |
| ATOM | 356 O LYS | | | 44.889 | | 1.00 26.75 | AAAA |
| | | 44 | 49.265 | 43.792 | 65.586 | 1.00 27.37 | AAAA |
| MOTA | 357 N GLU | 45 | 47.731 | 45.278 | 64.881 | 1.00 29.20 | |
| ATOM | 358 CA GLU | 45 | 46.580 | 44.414 | | 1.00 25.20 | AAAA |
| ATOM | 359 CB GLU | 45 | | | | 1.00 21.58 | AAAA |
| | | | 45.387 | 45.243 | | 1.00 18.24 | AAAA |
| ATOM | 360 CG GLU | 45 | 45.551 | 45.828 | 67.077 | 1.00 26.57 | AAAA |
| ATOM | 361 CD GLU | 45 | 44.418 | 46.772 | | 1.00 23.12 | |
| MOTA | 362 OE1 GLU | 45 | 44.224 | | | 1.00 23.12 | AAAA |
| ATOM | | | | 47.783 | 66.746 | 1.00 21.64 | AAAA |
| | | 45 | 43.725 | 46.509 | 68.454 | 1.00 26.48 | AAAA |
| MOTA | 364 C GLU | 45 . | 46.163 | 43.710 | 63.870 | 1.00 26.31 | |
| ATOM | 365 O GLU | 45 | 45.400 | 42.739 | | 3 00 20.31 | AAAA |
| MOTA | 366 N LEU | 46 | | | 63.889 | 1.00 22.32 | AAAA |
| | | | 46.674 | 44.204 | 62.748 | 1.00 20.15 | AAAA |
| MOTA | 367 CA LEU | 46 | 46.317 | 43.642 | 61.448 | 1.00 25.80 | AAAA |
| MOTA | 368 CB LEU | 46 | 46.137 | 44.774 | 60.433 | 1.00 27.25 | |
| ATOM | 369 CG LEU | 46 | 45.763 | | | | AAAA |
| ATOM | | | | 44.397 | 58.997 | 1.00 37.72 | AAAA |
| | | 46 | 44.356 | 43.810 | 58.984 | 1.00 39.46 | AAAA |
| ATOM | 371 CD2 LEU | 46 | 45.822 | 45.632 | 58.101 | 1.00 35.43 | |
| ATOM | 372 C LEU | 46 | 47.305 | 42.623 | | | AAAA |
| ATOM | 373 O LEU | | | | 60.896 | 1.00 28.88 | AAAA |
| | | 46 | 48.513 | 42.860 | 60.862 | 1.00 31.98 | AAAA |
| MOTA | 374 N ILE | 47 | 46.791 | 41.469 | 60.482 | 1.00 16.92 | AAAA |
| ATOM | 375 CA ILE | 47 | 47.638 | 40.448 | 59.872 | | |
| ATOM | 376 CB ILE | 47 | 47.412 | | | 1.00 20.98 | · AAAA |
| ATOM | | | | 39.046 | 67.513 | 1.00 21.51 | AAAA |
| | | 47 | 48.115 | 37.958 | 53.696 | 1.00 20.32 | AAAA |
| MOTA | 378 CG1 ILE | 47 | 47.947 | 39.040 | 6 .950 | 1.00 20.71 | |
| MOTA | 379 CD1 ILE | 47 | 49.450 | 39.207 | | | AAAA |
| ATOM | 380 C ILE | | | | 62.052 | 1.00 38.87 | AAAA |
| | | 47 | 47.227 | 40.417 | 58.406 | 1.00 24.50 | AAAA |
| MOTA | 381 O ILE | 47 | 46.036 | 40.279 | 58,101 | 1.00 20.74 | AAAA |
| ATOM | 382 N LYS | 48 | 48.195 | 40.550 | 57.500 | 1.00 18.73 | |
| ATOM | 383 CA LYS | 48 | | | | | AAAA |
| | | | 47.883 | 40.543 | 56.072 | 1.00 15.55 | AAAA |
| MOTA | 384 CB LYS | 48 | 49.095 | 40.991 | 55.239 | 1.00 16.52 | AAAA |
| ATOM | 385 CG LYS | 48 | 48836 | 41.011 | 53.738 | | |
| ATOM | 386 CD LYS | | | | | 1.00 23.25 | AAAA . |
| | | 48 | 50.072 | 41.451 | 52.957 | 1.00 32.69° | AAAA |
| MOTA | 387 CE LYS | 48 | 49.796 | 41.496 | 51.462 | 1.00 26.00 | AAAA |
| MOTA | 388 NZ LYS | 48 | 48.704 | 42.449 | 51.114 | 1.00 46.33 | |
| MOTA | 389 C LYS | 48 | | | | | AAAA |
| | , | | 47.473 | 39.140 | 55.629 | 1.00 14.43 | AAAA |
| ATOM | 390 O LYS | 48 | 48.177 | 38.174 | 55.887 | 1.00 16.83 | AAAA |
| ATCM | 391 N SER | 49 | 46.343 | 39.049 | 54.945 | 1.00 16.61 | |
| ATOM | 392 CA SER | 49 | 45.838 | | | | AAAA |
| ATOM | | | . | 37.780 | 54.439 | 1.00 14.33 | AAAA |
| | | 49 | | 37.984 | 53.694 | 1.00 13.21 | AAAA |
| ATOM | 394 OG SER | 49 | 43.509 | 38.613 | | 1.00 16.86 | AAAA |
| ATCM | 395 C SER | 49 | | 37.131 | 53 450 | | |
| ATOM | | | | | 53.459 | 1.00 24.11 | AAAA |
| AIUN | 396 O SER | 49 | 47.463 | 37.815 | 52.663 | 1.00 19.59 | AAAA |
| | | | | | • | | |

| | | | | 50 | 46.890 | 35.805 | 53.519 | 1.00 16.83 | AAAA |
|------|-------|------|-------|----------|--------|---------|--------------|--------------|--------|
| MOTA | 397 | N | ARG | 50 | 47.724 | 35.037 | | 1.00 23.88 | AAAA |
| ATOM | 398 | CA | ARG | 50 | | 34.247 | | 1.00 27.48 | AAAA |
| MOTA | 399 | | ARG | 50 | 48.805 | 33.036 | | 1.00 22.99 | AAAA |
| ATOM | 400 | CG | ARG | 50 | 48.284 | 32.263 | 54.759 | 1.00 25.20 | AAAA |
| ATOM | 401 | CD | ARG | 50 | 49.453 | 31.197 | 55.684 | 1.00 15.88 | AAAA |
| ATOM | 402 | NE | ARG | 50 | 49.073 | | 55.368 | 1.00 14.34 | AAAA |
| ATOM | 403 | CZ _ | ARG | 50 | 48.411 | 30.093 | | 1.00 15.78 | AAAA |
| ATOM | 404 | NH1 | ARG | 50 . | 48.023 | 29.863 | 54.117 | 1.00 16.78 | AAAA |
| ATOM | 405 | NH2 | ARG | 50 | 48.150 | 29.197 | 56.312 | 1.00 20.20 | AAAA |
| ATOM | 406 | С | ARG | 50 | 46.821 | 34.023 | 51.905 | | AAAA |
| ATOM | 407 | 0 | ARG | 50 - | 45.763 | 33.650 | 52.414 | 1.00 18.63 | AAAA |
| ATOM | 408 | N | PRO | 51 | 47.203 | 33.596 | 50.699 | 1.00 15.63 | AAAA |
| | 409 | CD | PRO | 51 | 48.322 | 34.028 | 49.850 | 1.00 19.45 | AAAA |
| MOTA | 410 | CA | PRO | 51 | 46.387 | .32:606 | 49.994 | 1.00 14.35 | AAAA |
| MOTA | 411 | CB | PRO | 51 | 47.076 | 32.514 | 48.629 | 1.00 17.73 | AAAA |
| MOTA | 412 | CG | PRO | 51 | 47.707 | | 48.475 | 1.00 17.62 | AAAA |
| ATOM | 413 | C | PRO | 51 | 46.452 | 31.256 | 50.708 | 1.00 15.73 | |
| ATOM | 414 | ō | PRO | 51 | 47.460 | 30.942 | | 1.00 18.67 | AAAA |
| ATOM | 415 | N | ALA | 52 | 45.377 | 30.470 | 50.618 | 1.00 11.47 | AAAA |
| MOTA | 416 | CA | ALA | 52 | 45.375 | 29.117 | 51.161 | 1.00 9.78 | AAAA |
| MOTA | | CB | ALA | 52 | 43.967 | 28.529 | 51.112 | 1.00 12.19 | AAAA |
| MOTA | 417 | | ALA | 52 | 46.301 | 28.342 | 50.209 | 1.00 17.19 | AAAA |
| MOTA | 418 | C | ALA | 52 | 46.307 | 28.609 | 49.006 | 1.00 16.46 | AAAA |
| ATOM | 419 | 0 | | 53 | 47.081 | 27.392 | 50.723 | 1.00 16.40 | AAAA |
| MOTA | 420 | N | THR | 53 | 47.952 | 26.615 | 49.843 | 1.00 16.32 | AAAA |
| MOTA | 421 | CA | THR | 53 | 49.109 | 25.959 | 50.612 | 1.00 15.82 | AAAA |
| MOTA | 422 | CB | THR | 53 | 48.582 | 25.016 | 51.559 | 1.00 16.25 | AAAA |
| MOTA | 423 | | THR | 53 53 | 49.923 | 27.030 | 51.336 | 1.00 14.34 | AAAA |
| ATOM | 424 | | THR | | 47.104 | 25.520 | 49.215 | 1.00 14.06 | AAAA |
| MOTA | 425 | C | THR | 53 53 | 46.012 | 25.241 | 49.690 | 1.00 17.87 | AAAA |
| MOTA | 426 | 0 | THR | 53 | 47.599 | 24.903 | 48.145 | 1.00 16.10 | AAAA |
| MOTA | 427 | N | LYS- | 54 | 46.848 | 23.832 | 47.492 | 1.00 19.00 | AAAA |
| MOTA | 428 | CA | LYS | 54 | 47.671 | 23.245 | | 1.00 22.92 | AAAA |
| MOTA | 429 | CB | LYS | 54 | 46.955 | 22.172 | 45.539 | 1.00 32.99 | AAAA |
| MOTA | 430 | .CG | LYS | 54 | 45.787 | 22.733 | 44.757 | 1.00 51.34 | AAAA |
| ATOM | 431 | CD | LYS | 54 | 46.244 | 23.565 | 43.561 | 1.00 64.17 | AAAA |
| MOTA | 432 | CE | LYS | 54 | 46.898 | 22.733 | 42.505 | 1.00 63.45 | AAAA |
| ATOM | 433 | NZ | LYS | 54 | 46.554 | 22.738 | 48.520 | 1.00 22.48 | AAAA . |
| MOTA | 434 | C | LYS | 54 | 45.463 | 22.158 | 48.555 | 1.00 19.97 | AAAA |
| MOTA | 435 | 0 | LYS | 54 | 47.536 | 22.465 | 49.364 | 1.00 25.65 | AAAA |
| ATOM | 436 | N | GLU | 55 | 47.389 | 21.432 | 50.383 | 1.00 25.08 | AAAA |
| MOTA | 437 | CA | GLU | 55 | 48.718 | 21.241 | 51.116 | 1.00 25.40 | AAAA |
| MOTA | 438 | CB | GLU | 55 55 | 48.703 | 20.185 | 52.199 | 1.00 48.95 | AAAA |
| MOTA | 439 | CG | GLU | 55 55 | 50.106 | 19.821 | 52.673 | 1.00 64.21 | AAAA |
| ATOM | 440 | CD | GLU | 55 | 50.220 | 19.033 | 53.640 | 1.00 62.38 | AAAA |
| ATOM | 441 | OE1 | | 55 | 51.093 | 20.311 | 52.073 | 1.00 58.22 | AAAA |
| ATOM | 42 | OE2 | | 55 | 46.273 | 21.773 | | 1.00 18.91 | AAAA |
| MOTA | .43 | C | GLU | 55 | 45.489 | 20.908 | | 1.00 17.43 | AAAA |
| ATOM | -,44 | 0 | GLU | 55 | 46.196 | 23.029 | | 1.00 16.80 | AAAA |
| ATOM | 445 | N | GLU | 56 | | 23.432 | | 1.00 17.24 | AAAA |
| MOTA | 446 | CA | GLU | 56 | 45.137 | 24.855 | | 1.00 16.15 | AAAA |
| MOTA | 447 | CB | GLU | 56 | 45.399 | 24.941 | | 1.00 14.41 | AAAA |
| ATOM | 448 | CG | GLU | 56 | 46.709 | 26.354 | | | AAAA |
| MOTA | 449 | CD | GLU | 56 , | 47.087 | 27.252 | | | AAAA |
| ATOM | 450 | | . GLU | 56 | 46.713 | 26.564 | | | AAAA |
| MOTA | 451 | OE2 | GLU | 56 | 47.773 | | | | AAAA |
| ATOM | 452 | С | GLU | 56 | 43.781 | | | | AAAA |
| ATOM | 453 | 0 | GLU | 56 | 42.799 | | | | AAAA |
| ATOM | 454 | N | LEU | 57 | 43.722 | | | | AAAA |
| ATOM | 455 | CA | LEU | 57 | 42.466 | 23.579 | | | AAAA |
| MOTA | 456 | CB | LEU | 57 | 42.591 | | | | AAAA |
| ATOM | 457 | CG | LEU | 57 | 42.773 | | | | AAAA |
| ATOM | 458 | | LEU | 57 | 42.923 | | | | AAAA |
| ATOM | 459 | | LEU | 57 | 41.546 | 26.380 | | | AAAA |
| ATOM | 460 | С | LEU | 57 | 42.016 | 22.126 | 49.868 | | AAAA |
| | 461 | _ | LEU | 57 | 40.824 | 21.82 | 3 . 49 . 972 | | AAAA |
| ATOM | 462 | N | LEU | 58 | 42.975 | 21.23 | 49.636 | , T.00 TO.45 | |
| ATOM | -, -, | | | • | | | | | |
| | | | | | | | | | |

| | 4.0 | | | | | | | | |
|-------|-----------------|----------|------------|------------|--------|--------|----------|-------------|--------|
| ATOM | 46. | | | | 42.662 | 19.822 | | | AAAA |
| MOTA | 46 | 4 CB LEU | 58 | | 43.788 | 19.113 | 48.727 | 1.00 16.09 | AAAA |
| MOTA | 46 | | | | 44.029 | | | | |
| | | | | | | | | | AAAA |
| MOTA | 466 | | .58 | | 45.221 | 18.982 | 46.680 | 1.00 31.92 | аааа |
| MOTA | 46 | CD2 LEU | 58 | | 42.786 | 19.549 | 46.469 | 1.00 34.38 | AAAA |
| MOTA | 468 | C LEU | 58 | | 42.339 | | | 1.00 21.19 | |
| | 469 | | | | | | | | AAAA |
| ATOM | | | 58 | | 42.067 | | 50.795 | 1.00 20.40 | AAAA |
| MOTA | 470 | N LEU | 59 | | 42.377 | 19.849 | 51.896 | 1.00 13.50 | `AAAA |
| MOTA | 471 | . CA LEU | 59 | | 41.958 | 19.261 | 53.173 | 1.00 15.58 | |
| ATOM | 472 | CB LEU | 59 | | 42.182 | | | | AAAA |
| | 473 | | | | | | 54.339 | 1.00 18.98 | AAAA |
| ATOM | | | 59 | | 43.619 | | . 54.774 | 1.00 22.57 | AAAA |
| ATOM | 474 | | 59 | | 43.640 | 21.654 | 55.808 | 1.00 19.88 | AAAA |
| MOTA | 475 | CD2 LEU | 59 | - | 44.255 | 19.253 | 55.339 | 1.00 26.71 | AAAA |
| ATOM | 476 | | 59 | | 40.446 | | 53.043 | | |
| | 477 | | | | | | | 1.00 17.55 | AAAA |
| MOTA | | | 59 | | 39.897 | | 53.724 | 1.00 18.02 | AAAA |
| MOTA. | 478 | N PHE | 60 - | | 39.766 | 19.737 | 52.179 | 1.00 14.64 | - AAAA |
| ATOM | 479 | CA PHE | 60 | | 38.338 | 19.536 | 51.970 | 1.00 18.17 | |
| ATOM | 480 | | 60 | | 37.519 | | | | AAAA |
| • | | | | | | 20.694 | 52.557 | 1.00 18.80 | AAAA |
| MOTA | 481 | CG PHE | 60 | | 36.028 | 20.564 | 52.316 | 1.00 15.94 | AAAA |
| MOTA | 482 | CD1 PHE | 60 | | 35.320 | 19.476 | 52.817 | 1.00 19.98 | AAAA |
| ATOM | 483 | CD2 PHE | 60 | | 35.339 | 21.524 | 51.576 | 1.00 18.09 | AAAA |
| MOTA | 484 | CE1 PHE | 60 | | 33.947 | | | | |
| | | | | | | 19.338 | 52.587 | 1.00 18.72 | AAAA |
| ATOM | 485 | CE2 PHE | 60 | | 33.964 | 21.399 | 51.338 | 1.00 19.19 | AAAA |
| ATOM | 486 | CZ PHE | 60 | | 33.268 | 20.295 | 51.850 | 1.00 18.43 | AAAA |
| ATOM | 487 | C PHE | 60 | | 37.916 | 19.337 | 50.510 | 1.00 16.45 | AAAA |
| ATOM | 488 | O PHE | 60 | | 37.227 | 18.371 | | | |
| | | | | | | | 50.179 | 1.00 19.18 | AAAA |
| MOTA | 489 | N HIS | 61 | | 38.308 | 20.257 | | 1.00 18.26 | AAAA |
| ATOM | 490 | CA HIS' | 61 | | 37.913 | 20.163 | 48.235 | 1.00 14.47 | AAAA |
| MOTA | 491 | CB HIS | 61 | | 38.004 | 21.545 | 47.582 | 1.00 17.15 | AAAA |
| MOTA | 492 | CG HIS | 61 | | 36.968 | 22.494 | 48.084 | 1.00 14.20 | AAAA |
| ATOM | 493 | CD2 HIS | 61 | - | | | | | |
| | | | | | 35.645 | 22.580 | 47.816 | 1.00 11.05 | AAAA |
| ATOM | 494 | ND1 HIS | 61 | | 37.237 | 23.477 | 49.012 | 1.00 23.25 | AAAA |
| MOTA | 495 | CE1 HIS | 6 1 | | 36.121 | 24.131 | 49.291 | 1.00 13.35 | AAA:A |
| ATOM | 496 | NE2 HIS | 61 | | 35.143 | 23.606 | 48.579 | 1.00 21.07 | AAAA |
| ATOM | 497 | C HIS | 61 | | 38.695 | | | | |
| | | | | | | 19.157 | 47.417 | 1.00 18.29 | AAAA |
| MOTA | 498 | O HIS | 61 | | 39.828 | 18.819 | 47.761 | 1.00 17.50 | AAAA |
| ATOM | 499 | n thr | 62 | | 38.071 | 18.658 | 46.346 | 1.00 15.39 | AAAA |
| MOTA | 500 | CA THR | 62 | | 38.741 | 17.686 | 45.473 | 1.00 19.02 | AAAA |
| MOTA | 501 | CB THR | 62 | | 37.734 | 16.767 | 44.756 | 1.00 19.61 | |
| | 502 | OG1 THR | 62 | | | | | | AAAA |
| MOTA | | | | | 36.795 | 17.548 | 44.006 | 1.00 22.05 | AAAA |
| ATOM | 503 | CG2 THR | 62 | | 36.995 | 15.925 | 45.767 | 1.00 28.99 | AAAA |
| MOTA | 504 | C THR | 62 | . . | 39.595 | 18.398 | 44.440 | 1.00 23.22 | AAAA |
| ATOM | 505 | O THR | 62 | _ | 39.311 | 19.532 | 44.044 | 1.00 17.47 | AAAA |
| ATOM | 506 | N GLU | 63 | | 40.657 | 17.732 | | | |
| | | | | | | | 44.009 | 1.00 18.94 | AAAA |
| ATOM | 507 | | 63 | | 41.571 | 18.324 | 43.046 | 1.00 22.44 | AAAA |
| MOTA | 508 | CB GLU | 63 | | 42.736 | 17.384 | 42.750 | 1.00 28.31 | AAAA |
| MOTA | 50 9 | CG GLU | 63 | | 43.885 | 17.476 | 43.708 | 1.00 60.37 | AAAA |
| MOTA | 510 | CD GLU | 63 | | 45.154 | 16.893 | 43.115 | 1.00 65.08 | AAAA |
| ATOM | 511 | OE1 GLU | 63 | | 45.603 | | | | |
| | | | | | | 17.407 | 42.065 | 1.00 66.44 | AAAA |
| ATOM | 512 | OE2 GLU | 63 | | 45.697 | 15.927 | 43.694 | 1.00 71.72 | AAAA |
| MOTA | 513 | C GLU | 63 | | 40.983 | 18.764 | 41.730 | 1.00 18.63 | AAAA |
| ATOM | 514 | O GLU | 63 | | 41.340 | 19.827 | 41.228 | 1.00 18.37 | AAAA |
| ATOM | 515 | N ASP | 64 | | 40.108 | 17.943 | 41.153 | | |
| | | | | | | | | 1.00 19.77 | AAAA |
| ATOM | 515 | CA ASP | 64 | | 39.508 | 18.277 | 39.864 | 1.00 -17.88 | AAAA |
| MOTA | 517 | CB ASP | 64 | | 38.584 | 17.159 | 39.372 | 1.00 20.43 | AAAA |
| ATOM | 518 | .CG ASP | 64 | | 37.429 | 16.884 | 40.330 | 1.00 42.71 | AAAA |
| ATOM | 519 | OD1 ASP | 64 | | 36.415 | 16.291 | 39.899 | 1.00 45.01 | |
| | 520 | OD2 ASP | | | | | 43 554 | | AAAA |
| ATOM | | | 64 | | 37.537 | 17.243 | 41.521 | 1.00 51.77 | AAAA |
| ATOM | 521 | C ASP | 64 | | 38.701 | 19.582 | 39.964 | 1.00 21.90 | AAAA |
| ATOM | 522 | O ASP | 64 . | | 38.726 | 20.410 | 39.042 | 1.00 17.35 | AAAA |
| ATOM | 523 | N TYR | 65 | | 37.980 | 19.750 | 41.072 | 1.00 16.17 | |
| | | | | | | | | | AAAA |
| ATOM | 524 | CA TYR | 65 | | 37.178 | 20.957 | 41.292 | 1.00 15.62 | . AAAA |
| ATOM | 525 | CB TYR | 65 | | 36.258 | 20.796 | 42.529 | 1.00 12.04 | AAAA |
| ATOM | 526 | CG TYR | 65 | | 35.501 | 22.065 | 42.886 | 1.00 12.23 | AAAA |
| ATOM | 527 | CD1 TYR | 65 | | 34.699 | 22.718 | 41.940 | 1.00 14.73 | |
| | | | | | | | 34.J4U | | AAAA |
| ATOM | 528 | CE1 TYR | 65 | | 34.028 | 23.910 | 42.253 | 1.00 18.23 | aaaa |

SUBSTITUTE SHEET (RULE 26)

| | | | | | 25 600 | 22.631 | 44.163 | 1.00 13.67 | AAAA |
|--------------|------------|--------|------------|----------------|------------------|------------------|----------------------|--------------------------|--------------|
| MOTA | 529 | CD2 | | 65 | 35.609 | 23.824 | 44.486 | 1.00 18.16 | AAAA |
| MOTA | 530 | | TYR | 65 | 34.943 | 24.461 | 43.533 | 1.00 16.88 | AAAA |
| ATOM | 531 | | TYR | 65. | 34.162 | | 43.837 | 1.00 14.59 | AAAA |
| ATOM | 532 | | TYR | 65 | 33.555 | 25.665 | 41.459 | 1.00 15.27 | AAAA |
| ATOM | 533 | С | TYR | 65 | 38.090 | 22.177 | 40.798 | 1.00 15.96 | AAAA |
| ATOM | 534 | 0 | TYR | 65 | 37.882 | 23.189 22.073 | 42.321 | 1.00 14.29 | AAAA |
| ATOM | 535 | N | ILE | 66 | 39.098 | | 42.540 | 1.00 18.86 | AAAA |
| ATOM | 536 | CA | ILE | 66 | 40.022 | 23.179 | 43.617 | 1.00 15.56 | AAAA |
| MOTA | 537 | CB | ILE | 66 | 41.090 | | 43.698 | 1.00 20.45 | AAAA |
| ATOM | 538 | CG2 | ILE | 66 | 42.152 | | 44.967 | 1.00 19.68 | AAAA |
| ATOM | 539 | CG1 | ILE | 66 | 40.405 | | 45.454 | 1.00 29.11 | · AAAA |
| MOTA | 540 | CD1 | ILE | 66 | 39.717 | 23.519 | 41.236 | 1.00 25.20 | AAAA |
| MOTA | 541 | C | ILE | 66 | 40,716 | 24.692 | 40.895 | 1.00 14.60 | AAAA |
| MOTA | 542 | 0 | ILE | 66 | 40.809 | | 40.498 | 1.00 18.21 | AAAA |
| MOTA | 543 | N | ASN | 67 | 41.190 | | 39.236 | 1.00 20.03 | AAAA |
| ATOM | 544 | CA | ASN | 67 | 41.879 | | 38.580 | 1.00 21.73 | AAAA |
| ATOM | 545 | CB | ASN | 67 | 42.448 | | 39.333 | 1.00 21.69 | AAAA |
| ATOM | 546 | CG | ASN | 67 | 43.645 | | 40.110 | 1.00 23.97 | AAAA |
| ATOM | 547 | | ASN | 67 | 44.293 | | 39.086 | 1.00 23.23 | AAAA |
| ATOM | 548 | ND2 | ASN | 67 | 43.947 | | 38.250 | 1.00 15.87 | AAAA |
| MOTA | 549 | C | ASN | 67 | 40.970 | | 37.473 | 1.00 18.64 | AAAA |
| ATOM | 550 | 0 | ASN | 67 | 41.431 | | 38.295 | 1.00 16.55 | AAAA |
| ATOM | 551 | N | THR | 68 | 39.681 | | 37.400 | 1.00 20.34 | AAAA |
| ATOM | 552 | CA | THR | 68 | 38.729 37.360 | | 37.441 | 1.00 22.99 | AAAA |
| MOTA | 553 | CB | THR | 68 | 37.511 | | 36.978 | 1.00 21.75 | AAAA |
| ATOM | 554 | | THR | 68 · 68 | 36.378 | | 36.536 | 1.00 17.37 | AAAA |
| MOTA | 555 | | THR | 68 | 38.561 | | 37.755 | 1.00 16.66 | AAAA |
| MOTA | 556 | C | THR THR | 68 | 38.472 | | 36.871 | 1.00 18.79 | AAAA AAAA |
| MOTA | 557 | N O | LEU | 69 | 38.534 | 4 25.604 | | 1.00 14.82 | AAAA |
| MOTA | 558 559 | CA | LEU | 69 | 38.40 | 5 27.000 | 39.447 | 1.00 15.20 1.00 16.87 | AAAA |
| MOTA | 560 | CB | LEU | 69 | 38.29 | 5 27.126 | | 1.00 14.76 | AAAA |
| ATOM ATOM | 561 | CG | LEU | 69 | 37.05 | | | 1.00 16.81 | AAAA |
| ATOM | 562 | | LEU | 69 | 37.21 | | | 1.00 17.26 | AAAA |
| ATOM | 563 | | LEU | 69 | 35.83 | 2 27.312 | | | AAAA |
| ATOM | 564 | C | LEU | 69 | 39.62 | | | 1.00 13.30 | AAAA |
| ATOM | 565 | 0 | LEU | 69 | 39.50 40.80 | | | 1.00 13.40 | AAAA |
| ATOM | 566 | N | MET | 70 | 40.00 | | | 1.00 16.97 | AAAA |
| MOTA | 567 | CA | MET | 70 70 | 43.25 | | 39.075 | 1.00 14.87 | AAAA |
| ATOM | . 568 | CB | MET | 70 70 | 43.33 | | 40.582 | 1.00 15.18 | AAAA |
| MOTA | 569 | CG | MET | 70 | 44.82 | | | 1.00 28.71 | AAAA AAAA |
| ATOM | 570 | SD | MET MET | 70 | 46.05 | 1 27.228 | | | AAAA |
| MOTA | 571 | CE | MET | 70 | 42.06 | 4 28.119 | 37.155 | 1.00 19.11 | AAAA |
| MOTA | 572 | С О | MET | 70 | 42.49 | 8 29.170 | | | AAAA |
| ATOM | 573 574 | N | GLI | 71 | 41.64 | 8 27.118 | | | AAAA |
| ATOM | 575 | CA | GLU | 71 | 41.65 | 1 27.226 | | | AAAA |
| ATOM | 576 | CB | GLi | 71 | 41.39 | 7 25.85 | | | AAAA |
| MOTA | 577 | | GLU | 71 | 41.38 | 7 25.88 | | | AAAA |
| MOTA MOTA | 578 | CD | GLU | 71 | 42.78 | 25.92 | 0 32.193 1 30.958 | | AAAA |
| ATOM | 579 | | l GLU | 71 | 42.89 | | | | AAAA |
| MOTA | 580 | | 2 GLU | 71 | 43.76 | | | 16 10 | AAAA |
| ATOM | 581 | | GLU | 71 | 40.58 | | | 1.00 17.20 | AAAA |
| ATOM | . 582 | | GLU | 71 | 40.83 | | | 7 1.00 15.68 | AAAA |
| ATOM | 583 | N | ALA | 72 | 39.38 | | | 4 1.00 16.07 | AAAA |
| MOTA | 584 | | | 72 | 38.30 37.03 | | | 5 1.00 17.21 | AAAA |
| ATOM | 585 | | | 72 | 38.6 | | | 7 1.00 19.07 | AAAA |
| ATOM | 586 | | λLA | 72 | 38.44 | | | 4 1.00 15.92 | AAAA |
| MOTE | 587 | | ALA | 72 73 | 39.20 | | - | 2 1.00 15.86 | AAAA |
| MOTA | 588 | | GLU | 73 73 | 39.6 | | 7 36.37 | 2 1.00 15.50 | AAAA |
| MOTA | 589 | | | 73 73 | 40.0 | | 0 37.82 | 8 1.00 14.12 | AAAA |
| ATOM | 590 | | | 73 73 | 40.4 | | 5 38.21 | | AAAA |
| MOTA | 591 | | | 73 73 | 40.9 | | 9 39.62 | 9 1.00 17.23 | AAAA AAAA |
| ATOM | 592 | | 1 GLU | 73 | 40.1 | 47 33.69 | 6 40.57 | 3 1.00 18.51 | AAAA AAAA |
| MOTE | 593 | | 2 GLU | 73 | 42.2 | | 39.79 | 3 1.00 20.88 | · nnnn |
| MOTA | 594 | , UE | . 300 | - - | - | | | | |
| • | | | | | - | un P oo | | • | |
| | | | | | / | | _ | | |

| _ | | | | | | | | | |
|--------------|------------|-----------|------------------|--------------------------|------------------|------------------|------------------|--------------------------|----------------|
| ATOM | 59 | | | 73 | 40.70 | 32.70 | 9 35.495 | 1.00 20.36 | AAAA |
| MOTA | 590 | | | | 40.52 | | 6 34.948 | 1.00 17.74 | AAAA |
| MOTA MOTA | 59° 598 | | ARG A ARG | | 41.832 | | | | AAAA |
| ATOM | 599 | | | | 42.911 44.256 | | | | AAAA |
| ATOM | 600 | | | | 44.365 | | | | AAAA |
| MOTA | 601 | l C | D ARG | 74 | 45.723 | | | | AAAA AAAA |
| MOTA | 602 | | | 74 | 45.918 | 28.696 | 33.950 | | AAAA |
| MOTA MOTA | 603 604 | | | . 74 | 46.439 | | | | AAAA |
| ATOM | 605 | | H1 ARG H2 ARG | 74 74 | 46.843 46.466 | | | | AAAA |
| ATOM | 606 | | | 74 | 42.643 | | | | AAAA |
| ATOM | - 607 | | | 74 | 43.148 | | | 1.00 15.41 | AAAA AAAA |
| ATOM | 608 | | | 75 | 41.859 | | | | AAAA |
| MOTA MOTA | 609 610 | | | 75 75 | 41.544 | | | | AAAA |
| MOTA | 611 | | | 75 75 | 41.474 43.047 | | | | AAAA |
| MOTA | 612 | | CYS | 75 | 40.216 | | | 1.00 19.30 1.00 15.81 | AAAA |
| MOTA | 613 | 0 | CYS | 75 | 39.762 | | | 1.00 13.81 | AAAA AAAA |
| ATOM | 614 | | GLN | 76 | 39.601 | 32.959 | 32.007 | | AAAA |
| ATOM ATOM | 615 616 | | | 76 76 | 38.339 | 33.686 | | 1.00 23.22 | AAAA |
| ATOM | 617 | | | 76 76 | 38.595 37.564 | 35.122 36.107 | | 1.00 22.99 | AAAA |
| ATOM | 618 | CI | | 76 | 37.588 | 36.229 | | 1.00 44.69 1.00 47.78 | AAAA |
| MOTA | 619 | | 1 GLN | 76 | 37.563 | 35.228 | | 1.00 62.95 | AAAA AAAA |
| MOTA | 620 | | 2 GLN | 76 | 37.619 | 37.452 | | 1:00 45.96 | AAAA |
| MOTA MOTA | 621 622 | 0 | GLN GLN | 76 76 | 37.304 | 32.975 | | 1.00 23.43 | AAAA |
| ATOM | 623 | N | CYS | 77 | 36.826 36.951 | 33.512 31.754 | 30.135 31.521 | 1.00 19.93 1.00 15.97 | AAAA |
| MOTA | 624 | CA | CYS | . 7 7 | 36.004 | 30.979 | 30.741 | 1.00 13.97 | AAAA AAAA |
| ATOM | 625 | CB | | 77 | 36.738 | 30.225 | 29.623 | 1.00 24.64 | AAAA |
| ATOM ATOM | 626 627 | SG C | CYS CYS | 7 7 7 7 | 37.848 | 28.887 | 30.269 | 1.00 25.26 | AAAA |
| ATOM | 628 | Ö | CYS | 7 7 | 35.302 35.685 | 29.951 29.702 | 31.594 32.732 | 1.00 19.68 1.00 20.02 | AAAA |
| MOTA | 629 | N | VAL | 78 | 34.254 | 29.366 | 31.022 | 1.00 20.02 | AAAA AAAA |
| MOTA | 630 | CA | VAL | 78 | 33.531 | 28.288 | 31.671 | 1.00 18.73 | AAAA |
| ATOM ATOM | 631 632 | CB CG: | VAL 1 VAL | 78 78 | 32.016 | 28.455 | 31.557 | 1.00 15.57 | AAAA |
| ATOM | 633 | | VAL | 78 | 31.312 31.603 | 27.304 29.792 | 32.262 32.151 | 1.00 21.27 | AAAA |
| ATOM | 634 | С | VAL | 78 | 33.950 | 27.077 | 30.859 | 1.00 19.47 1.00 24.02 | AAAA . AAAA |
| MOTA | 635 | 0 | VAL | 78 | 33.499 | 26.894 | 29.718 | 1.00 24.08 | AAAA |
| MOTA | 636 | N | PRO | 79 | 34.848 | 26.249 | 31.420 | 1.00 18.91 | AAAA |
| ATOM ATOM | 637 638 | CD | PRO PRO | 79 79 | 35.470 35.320 | 26.341 | 32.756 | 1.00 17.70 | AAAA |
| ATOM | 639 | СВ | PRO | 79 | 36.295 | 25.056 24.432 | 30.720 31.732 | 1.00 23.37 1.00 21.92 | AAAA AAAA |
| MOTA | 640 | CG | PRO | 79 | 36.802 | 25.677 | 32.498 | 1.00 20.90 | AAAA |
| MOTA | 641 | C | PRO | 79 | 34.152 | 24.144 | 30.376 | 1.00 27.44 | AAAA |
| MOTA MOTA | 642 643 | O N | PRO LYS | 79 80 | 33.177 34.245 | 24.064 | 31.119 | 1.00 22.20 | Aaaa |
| ATOM | 644 | CA | LYS | 80 | 33.212 | 23.488 22.570 | 29.224 28.775 | 1.00 23.35 1.00 26.78 | AAAA |
| ATOM | 645 | CB | LYS | 80 | 33.708 | 21.853 | 27.518 | 1.00 20.78 | AAAA AAAA |
| MOTA | 646 | CG | LYS | 80 | 35.098 | 21.256 | 27.680 | 1.00 51.34 | ΆλλΑ |
| MOTA | 647 648 | CD | LYS | 80 | 35.669 | 20.817 | 26.336 | 1.00 68.70 | AAAA |
| MOTA MOTA | 649 | NZ CE | LYS LYS | 80 80 | 37.131 37.688 | 20.401 | 26.451 | 1.00 70.04 | AAAA |
| ATOM | 650 | c | LYS | 80 | 32.875 | 19.949 21.571 | 25.141 29.875 | 1.00 73.72 1.00 24.71 | AAAA AAAA |
| ATOM | 651 | 0 | LYS | 80 | 33.770 | 20.957 | 30.458 | 1.00 24.23 | AAAA |
| MOTA | | N | GLY | 81 | 31.582 | 21.431 | 30.161 | 1.00 16.74 | AAAA |
| MOTA MOTA | | CY | GLY | 81 91 | 31.126 | 20.509 | 31.194 | 1.00 18.96 | AAAA |
| MOTA MOTA | | С 0 | .GLY GLY | 81 81 | 31.151 30.604 | 21.039 20.396 | 32.630 | 1.00 22.38 | AAAA |
| MOTA | | N | ALA | 82 | 31.754 | 22.202 | 33.527 32.863 | 1.00 19.29 1.00 22.57 | аааа Аааа |
| MOTA | 657 | CA | ALA | 82 | 31.858 | 22.738 | 34.235 | 1.00 20.65 | алал Алаа |
| · MOTA | | CB | ALA | 82 | | 23.704 | 34.333 | 1.00 20.41 | AAAA |
| MOTA | | С 0 | ALA | 82 82 | 30.610 | 23.425 | 34.781 | 1.00 21.81 | AAAA |
| MOTA | 000 | ٠. | ALA | 82 | 30.425 | 23.529 | 35.994 | 1.00 16.95 | AAAA . |

SUBSTITUTE SHEET (RULE 26)

| MOTA | 661 | N | ARG | 83 | 29.758 | 23.926 | 33.897 | 1.00 17.68 | AAAA AAAA |
|--------------|------------|----------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 662 | CA | ARG | 83 | 28.549 | 24.596 | 34.360 | 1.00 15.04 1.00 21.02 | AAAA |
| MOTA | 663 | CB | ARG | 83 | 27.777 | 25.188 26.395 | 33.176 33.528 | 1.00 36.77 | AAAA |
| MOTA | 664 | CG | ARG | 83 | 26.938 26.061 | 26.353 | 34.729 | 1.00 41.28 | AAAA |
| ATOM | 665 | CD | ARG | 83 | 25.366 | 27.393 | 35.105 | 1.00 40.05 | AAAA |
| ATOM | 666 | NE | ARG | 83 83 | 24.530 | 27.492 | 36.134 | 1.00 51.15 | AAAA |
| ATOM | 667 | | ARG ARG | 83 | 24.286 | 26.432 | 36.893 | 1.00 55.10 | AAAA |
| MOTA | 668 669 | NH2 | | 83 | 23.931 | 28.646 | 36.399 | 1.00 54.26 | AAAA |
| ATOM | 670 | C | ARG | 83 | 27.701 | 23.530 | 35.030 | 1.00 21.33 | AAAA |
| ATOM ATOM | 671 | ŏ | ARG | 83 - | 27.193 | 23.708 | 36.130 | 1.00 24.88 | AAAA |
| ATOM | 672 | N | GLU | 84 | 27.565 | 22.406 | 34.352 | 1.00 18.76 | AAAA |
| ATOM | 673 | CA | GLU | 84 | 26.768 | 21.299 | 34.859 | 1.00 24.12 | AAAA AAAA |
| ATOM | 674 | CB | GLU | 84 | 26.527 | 20.290 | 33.744 | 1.00 32.64 1.00 37.91 | AAAA |
| ATOM | 675 | CG | GLU | 84 | 27.769 | 19.994 | 32.925 31.612 | 1.00 51.24 | AAAA |
| MOTA | 676 | CD | GLU. | 84 | 27.832 27.585 | 20.784 20.152 | 30.545 | 1.00 24.82 | AAAA |
| MOTA | 677 | | GLU | | 28.114 | 22.018 | 31.650 | 1.00 22.57 | AAAA |
| MOTA | 678 | OE2 | GLU | 84 84 | 27.394 | 20.570 | 36.043 | 1.00 25.36 | AAAA |
| ATOM | 679 | С 0 | GLU | 84 | 26.739 | 20.321 | 37.057 | 1.00 26.17 | AAAA |
| MOTA | 680 681 | N | LYS | 85 | 28.665 | 20.232 | 35.897 | 1.00 18.78 | AAAA |
| MOTA | 682 | CA | LYS | 85 | 29.399 | 19.497 | 36.915 | 1.00 20.03 | AAAA |
| MOTA MOTA | 683 | CB | LYS | 85 | 30.658 | 18.900 | 36.280 | 1.00 18.59 | AAAA AAAA |
| MOTA | 684 | CG | LYS | 85 | 31.603 | 18.223 | 37.268 | 1.00 35.69 | AAAA |
| ATOM | 685 | CD | LYS | 85 | 31.151 | 16.832 | 37.644 | 1.00 51.51 1.00 59.18 | AAAA |
| ATOM | 686 | CE | LYS | 85 | 31.451 | 15.864 15.858 | 36.520 36.240 | 1.00 56.63 | AAAA |
| ATCM | 687 | NZ | LYS | 85 | 32.914 29.811 | 20.263 | 38.181 | 1.00 18.31 | AAAA |
| ATOM | 688 | C | LYS | 85 85 | 29.696 | 19.738 | 39.290 | 1.00 21.65 | AAAA |
| MOTA | 689 | O N | LYS TYR | 86 | 30.274 | 21.495 | 38.012 | 1.00 19.45 | AAAA |
| MOTA | 690 691 | CA | TYR | | 30.776 | 22.272 | 39.145 | 1.00 14.26 | AAAA |
| ATOM ATOM | 692 | СВ | TYR | 86 | 32.207 | 22.692 | 38.840 | 1.00 14.95 | AAAA |
| ATOM | 693 | CG | TYR | 86 | 33.107 | 21.508 | 38.585 | 1.00 19.76 1.00 18.83 | AAAA AAAA |
| ATOM | 694 | CD1 | TYR | 8 6 | 33.384 | 20.591 | 39.601 | 1.00 20.29 | AAAA |
| ATOM | 695 | CE1 | | 86 | 34.247 | 19.519 | 39.388 37.337 | 1.00 18.14 | AAAA |
| ATOM | 696 | CD2 | | 86 | 33.711 34.567 | 21.322 20.261 | 37.112 | 1.00 22.66 | AAAA |
| MOTA | 697 | CE2 | | 86 86 | 34.832 | 19.364 | 38.145 | 1.00 22.61 | AAAA |
| ATOM | 698 | CZ OH | TYR TYR | 86 | 35.680 | 18.317 | 37.921 | 1.00 23.68 | AAAA |
| MOTA | 699 700 | C | TYR | 86 | 29.967 | 23.493 | 39.526 | 1.00 19.03 | AAAA |
| ATOM | 701 | Ö | TYR | 86 | 30.353 | 24.226 | 40.450 | 1.00 19.18 | AAAA |
| MOTA MOTA | 702 | N | ASN | 87 | 28.873 | 23.721 | 38.803 | 1.00 17.59 | AAAA AAAA |
| ATOM | 703 | ÇA | ASN | 87 | 27.953 | 24.843 | 39.071 | 1.00 18.07 1.00 23.87 | AAAA |
| ATCM | 704 | CB | ASN | 87 | 27.413 | 24.730 | 40.514 40.688 | 1.00 30.67 | AAAA: |
| ATOM | 705 | CG | ASN | 87 | 26.020 | 25.349 25.520 | 41.819 | 1.00 31.55 | AAAA |
| ATOM | 706 | | ASN | 87 | 25.531 25.370 | 25.661 | 39.580 | 1.00 20.18 | AAAA |
| ATOM | 707 | ND2 | asn asn | 87 · 87 | 28.641 | 26.197 | 38.875 | 1.00 24.24 | AAAA |
| ATOM | 708 709 | С 0 | ASN | 87 | 28.283 | 27.190 | 39.519 | 1.00 18.57 | AAAA |
| ATOM | 710 | Ŋ | ILE | 88 | 29.617 | 26.237 | 37.970 | 1.00 18.80 | AAAA AAAA |
| MOTA MOTA | 711 | CA | ILE | 88 | 30.353 | 27.471 | 37.680 | 1.00 18.55 | AAAA |
| ATOM | 712 | CB | ILE | 88 | 31.865 | 27.166 | 37.508 | 1.00 26.44 1.00 43.71 | AAAA |
| ATCM | 713 | | ILE | 88 | 32.613 | 28.406 | 37.044 | 1.00 36.30 | AAAA |
| ATCM | .714 | | ILE | 88 | 32.439 | 26.703 | 38.835 39.888 | 1.00 24.08 | AAAA |
| ATOM | 715 | | ILE | 88 | 32.295 29.887 | 27.735 28.142 | 36.392 | 1.00 14.36 | AAAA |
| ATOM | 716 | C | ILE | 88 | 29.584 | 27.459 | 35.426 | 1.00 21.93 | AAAA |
| atom | 717 | 0 | ILE | 88 89 | 29.843 | 29.473 | 36.380 | 1.00 18.71 | AAAA |
| ATCM | 718 | N | GLY GLY | 89 | 29.479 | 30.162 | 35.154 | 1.00 20.23 | AAAA |
| ATOM | 719 | CA C | GLY | 89 | 28.147 | 30.873 | 35.106 | 1.00 20.85 | AAAA |
| atom | 720 721 | 0 | GLY | 89 | 28.006 | 31.817 | 34.330 | 1.00 25.47 | AAAA |
| ATOM | 722 | N | GLY | 90 | 27.172 | 30.414 | 35.889 | 1.00 21.17 | AAAA CAAA |
| atom atom | 723 | CA | GLY | 90 | 25.863 | 31.060 | 35.898 | 1.00 24.44 | AAAA AAAA |
| ATOM | 724 | C | GLY | 90 | 25.862 | 32.371 | 36.668 | 1.00 30.60 1.00 28.13 | AAAA |
| ATCM | 725 | 0 | GLY | 90 | 26.900 | 32.788 | 37.168 36.755 | | AAAA |
| ATCM | 726 | N | TYR | 91 | 24.708 | 33.036 | 30.733 | 1.00 25.50 | • |
| • | | | • | | | | | | |

| | 707 | | | | | | |
|--------|-----------|---------|----------|------------|----------|------------|--------|
| ATOM | 727 CA | | 91 24. | 598 34.29 | 9 37.490 | 1.00 28.48 | |
| MOTA | 728 CB | TYR | 91 23. | 144 34.75 | | 1.00 29.88 | AAAA |
| ATOM | 729 CG | TYR | | 923 35.89 | | 1.00 29.88 | AAAA |
| MOTA | 730 CD | 1 TYR | | | | 1.00 33.88 | AAAA |
| ATOM | | 1 TYR | | | | 1.00 39.69 | AAAA |
| ATOM- | | _ | | 130 38.25 | | 1.00 31.76 | AAAA |
| | | | | 317 35.67 | | 1.00 40.63 | AAAA |
| ATOM | | | | 115 36.72 | 0 40.664 | 1.00 37.07 | |
| ATOM | 734 CZ | | 91 22. | 521 38.00 | 2 40.327 | 1.00 36.22 | AAAA |
| ATOM | 735 он | TYR | 91 22. | 306 39.03 | | 1.00 30.22 | AAAA |
| ATOM | 736 C | -TYR | 91 25. | | 7 30 037 | 1.00 44.71 | AAAA |
| ATOM | 737 o | | 91 25. | | 7 38.937 | 1.00 23.59 | AAAA |
| ATOM | 738 N | | 92 24. | | | 1.00 22.64 | AAAA |
| MOTA | 739 CA | | 22 25. | | | 1.00 23.09 | AAAA |
| | | | | | | 1.00 26.61 | AAAA |
| ATOM | 740 CB | | 24. | 289 31.47 | 6 41.306 | 1.00 32.57 | AAAA |
| MOTA | 741 CG | | 24. | 595 30.89 | | 1.00 41.38 | |
| ATOM | 742 CD | GLU 9 | 23.0 | | | 1.00 49.02 | AAAA |
| ATOM | 743 OE1 | . GLU 9 | 2 24.0 | 008 28.829 | | | - Aaaa |
| ATOM | 744 OE2 | | 2 22.4 | | | 1.00 45.51 | AAAA |
| MOTA | 745 C | | | | | 1.00 38.16 | AAAA |
| ATOM | 746 0 | | | | | 1.00 25.78 | AAAA |
| | | - | 2 27.0 | | 3 42.125 | 1.00 24.95 | AAAA |
| ATOM | | | 3 . 27.2 | | | 1.00 21.41 | AAAA |
| ATOM | 748 CA | | 3 28.6 | 74 31.519 | 40.777 | 1.00 21.14 | |
| ATOM | 749 CB | ASN 9 | 3 28.8 | 76 30.075 | | 1.00 17.27 | AAAA |
| MOTA | 750 CG | ASN 9 | 3 27.9 | | | 1.00 17.27 | AAAA |
| ATOM | 751 OD1 | ASN 9 | | | | 1.00 15.34 | AAAA |
| ATOM | 752 ND2 | ASN 9 | | | | 1.00 20.33 | AAAA |
| ATOM | 753 C | ASN 9 | | | | 1.00 20.49 | AAAA |
| ATOM | 754 O | ASN 9 | | | | 1.00 22.25 | AAAA |
| ATOM | 755 N | | | | | 1.00 20.29 | AAAA |
| ATOM | _ | | | | 39.045 | 1.00 25.45 | AAAA |
| | | PRO 94 | | | 39.839 | 1.00 23.03 | AAAA |
| ATOM | 757 CA | PRO 94 | | | | 1.00 23.05 | AAAA |
| ATOM | 758 CB | PRO 94 | 29.6 | 69 35.004 | 37.759 | 1.00 28.71 | |
| ATOM | 759 CG | PRO 94 | 28.5 | | | 1.00 40.02 | AAAA |
| ATOM | 760 C | PRO 94 | | | 37.697 | 1.00 40.02 | AAAA |
| MOTA | 761 O | PRO 94 | | 32 33.185 | | 1.00 26.51 | AAAA |
| ATOM | | VAL 95 | | | 38.688 | 1.00 17.36 | AAAA |
| ATOM | | VAL 95 | | | 36.478 | 1.00 21.12 | AAAA |
| ATOM | | | | | 36.281 | 1.00 17.00 | AAAA |
| ATOM | | - | | | 34.796 | 1.00 25.15 | AAAA |
| | | - | | | 34.533 | 1.00 27.19 | AAAA |
| ATOM | 766 CG2 | | 33.55 | 1 31.791 | 34.443 | 1.00 17.37 | AAAA |
| ATOM | | VAL 95 | 33.98 | 9 34.899 | 36.686 | 1.00 17.42 | AAAA |
| MOTA | | VAL 95 | 33.42 | 6 35.894 | 36.237 | 1.00 23.43 | |
| ATOM | 769 N S | SER 96 | 34.98 | | 37.563 | | AAAA |
| MOTA | 770 CA S | SER 96 | 35.56 | | | 1.00 18.84 | AAAA |
| ATOM | 771 CB 5 | SER 96 | 34.60 | | | 1.00 21.77 | AAAA |
| MOTA | | SER 96 | 34.72 | | | 1.00 23.11 | AAAA |
| ATOM | | SER 96 | | | | 1.00 24.43 | AAAA |
| ATOM | | ER 96 | 36.83 | | 38.789 | 1.00 29.09 | AAAA |
| ATOM | - | | 37.11 | | | 1.00 27.12 | AAAA |
| | | | , 37.61 | | 39.124 | 1.00 17.51 | AAAA |
| MOTA | | YR 97 | 38.80 | | | 1.00 20.69 | AAAA |
| ATOM | | 'YR 97 | 39.86 | 5 37.835 | | 1.00 21.82 | AAAA |
| ATOM | | YR 9.7 | 40.49 | | | 1.00 22.72 | |
| ATOM | 779 CD1 T | YR 97 | 39.93 | | | 1.00 28.47 | AAAA |
| MOTA | 780 CE1 T | YR 97 | 40.47 | | | | AAAA |
| ATOM | 781 CD2 T | YR 97 | 41.599 | | | 1.00 24.45 | AAAA |
| ATOM | 782 CE2 T | | | | | L:00 19.74 | AAAA |
| | | | 42.144 | | 36.832 | 1.00 21.63 | AAAA |
| MOTA | | YR 97 | 41.578 | | 35.759 1 | 1.00 23.13 | AAAA |
| MOTA | | YR 97 | 42.122 | | 34.501 1 | 00 28.54 | AAAA |
| MOTA | | YR 97 | 38.510 | 36.515 | | .00 20.12 | AAAA |
| MOTA | | YR 97 | 39.413 | | | 00 19.76 | |
| MOTA | 787 N AI | LA 98 | 37.243 | | | | AAAA |
| ATCM | 788 CA AL | | 36.899 | | | 00 18.56 | AAAA |
| MOTA | 789 CB AL | | 35.561 | | | .00 22.23 | AAAA |
| · MOTA | 790 C AL | | | | | .00 27.92 | AAAA |
| | | | 36.776 | | 43.224 1 | .00 23.56 | AAAA |
| MOT | | | 36.931 | | 44.289 1 | .00 20.14 | AAAA |
| TOM | 792 N ME | T 99 | 36.538 | 34.094 | | .00 16.84 | AAAA |
| | • | • | | | | | |

Figure 16-13

| | | | ` | 99 | 36.295 | 32.643 | 42.117 | 1.00 17.60 | AAAA |
|------|-----|--------|-----|-----|--------|--------|------------------|------------|------|
| ATOM | 793 | | MET | 99 | 35.864 | 32.137 | 40.736 | 1.00 17.05 | AAAA |
| MOTA | 794 | | MET | | 36.999 | 31.824 | 39.793 | 1.00 11.16 | AAAA |
| MOTA | 795 | CG | MET | 99 | | 31.698 | 38.113 | 1.00 16.54 | AAAA |
| ATOM | 796 | SD | MET | 99 | 36.314 | 30.295 | 38.312 | 1.00 17.83 | AAAA |
| ATOM | 797 | | MET | 99 | 35.165 | 31.800 | 42.650 | 1.00 18.98 | AAAA |
| MOTA | 798 | С | MET | 99 | 37.432 | | 43.251 | 1.00 18.21 | AAAA |
| ATOM | 799 | 0 | MET | 99 | 37.197 | 30.753 | 42.420 | 1.00 12.87 | AAAA |
| MOTA | 800 | N | PHE | 100 | 38.670 | 32.216 | | 1.00 17.13 | AAAA |
| MOTA | 801 | CA | PHE | 100 | 39.774 | 31.439 | 42.987 | 1.00 17.13 | AAAA |
| MOTA | 802 | CB | PHE | 100 | 40.559 | 30.681 | 41.917 | 1.00 15.20 | AAAA |
| ATOM | 803 | CG | PHE | 100 | 41.647 | 29.834 | 42.492 | | AAAA |
| ATOM | 804 | CD1 | PHE | 100 | 41.342 | 28.638 | 43.140 | 1.00 22.96 | AAAA |
| ATOM | 805 | CD2 | | 100 | 42.972 | 30.282 | 42.488 | 1.00 17.12 | |
| | 806 | CE1 | | 100 | 42:341 | 27.901 | | 1.00 19.23 | AAAA |
| MOTA | 807 | CE2 | | 100 | 43.974 | 29.552 | 43.129 | 1.00 16.99 | AAAA |
| MOTA | 808 | CZ | PHE | 100 | 43.658 | 28.360 | 43.779 | 1.00 17.78 | AAAA |
| ATOM | 809 | c | PHE | 100 | 40.755 | 32.305 | 43.774 | 1.00 20.54 | AAAA |
| ATOM | 810 | ō | PHE | 100 | 41.088 | 31.990 | 44.912 | 1.00 21.45 | AAAA |
| MOTA | 811 | И | THR | 101 | 41.219 | 33.401 | 43.187 | 1.00 18.02 | AAAA |
| ATOM | | | THR | 101 | 42.177 | 34.245 | 43.902 | 1.00 15.25 | AAAA |
| MOTA | 812 | CA | THR | 101 | 42.715 | 35.341 | 42.976 | 1.00 16.33 | AAAA |
| MOTA | 813 | CB | | 101 | 43.386 | 34.720 | 41.870 | 1.00 16.01 | AAAA |
| MOTA | 814 | | THR | 101 | 43.706 | 36.226 | 43.697 | 1.00 16.31 | AAAA |
| ATOM | 815 | CG2 | THR | 101 | 41.567 | 34.860 | 45.160 | 1.00 14.12 | AAAA |
| ATOM | 816 | C | THR | 101 | 42.110 | 34.707 | 46.244 | 1.00 16.86 | AAAA |
| MOTA | 817 | 0 | THR | 102 | 40.435 | 35.541 | 45.008 | 1.00 13.77 | AAAA |
| MOTA | 818 | N | GLY | | 39.770 | 36.145 | 46.156 | 1.00 16.29 | AAAA |
| MOTA | 819 | CA | GLY | 102 | 39.330 | 35.065 | 47.133 | 1.00 16.75 | AAAA |
| ATOM | 820 | C | GLY | 102 | 39.502 | 35.202 | 48.338 | 1.00 14.48 | AAAA |
| MOTA | 821 | 0 | GĹY | 102 | 38.752 | 33.986 | 46.615 | 1.00 16.24 | AAAA |
| MOTA | 822 | N | SER | 103 | 38.315 | 32.890 | 47.488 | 1.00 16.72 | AAAA |
| MOTA | 823 | CA | SER | 103 | 37.567 | 31.821 | 46.684 | 1.00 15.97 | AAAA |
| ATOM | 824 | CB | SER | 103 | | 32.349 | 46.197 | 1.00 26.86 | AAAA |
| ATOM | 825 | OG | SER | 103 | 36.339 | 32.264 | 48.218 | 1.00 17.88 | AAAA |
| MOTA | 826 | С | SER | 103 | 39.494 | 31.974 | 49.419 | 1.00 14.17 | AAAA |
| MOTA | 827 | 0 | SER | 103 | 39.405 | 32.057 | 47.515 | 1.00 11.40 | AAAA |
| ATOM | 828 | N | SER | 104 | 40.604 | 31.484 | 48.181 | 1.00 17.61 | AAAA |
| ATOM | 829 | CA | SER | 104 | 41.780 | | 47.160 | 1.00 15.89 | AAAA |
| ATOM | 830 | CB | SER | 104 | 42.888 | 31.206 | 46.362 | 1.00 27.82 | AAAA |
| ATOM | 831 | OG | SER | 104 | 42.525 | 30.102 | 49.271 | 1.00 17.02 | AAAA |
| ATOM | 832 | С | SER | 104 | 42.332 | 32.404 | 50.286 | 1.00 15.37 | AAAA |
| ATOM | 833 | 0 | SER | 104 | 42.867 | 31.958 | 49.052 | 1.00 17.10 | AAAA |
| ATOM | 834 | N | LEU | 105 | 42.206 | 33.698 | 50.016 | 1.00 16.95 | AAAA |
| ATOM | 835 | CA | LEU | 105 | 42.709 | 34.652 | | 1.00 18.44 | AAAA |
| ATOM | 836 | CB · | LEU | 105 | 42.728 | 36.037 | 49.365 49.981 | 1.00 29.88 | AAAA |
| ATOM | 837 | CG | LEU | 105 | 43.613 | 37.108 | | 1.00 20.25 | AAAA |
| ATOM | 838 | CD1 | LEU | 105 | 45.086 | 36 631 | 49.959 | 1.00 29.39 | AAAA |
| ATOM | 839 | CD2 | LEU | 105 | 43.438 | 38 418 | 49.175 | 1.00 14.81 | AAAA |
| ATOM | 840 | С | LEU | 105 | 41.837 | 34 637 | 51.282 | 1.00 17.74 | AAAA |
| ATOM | 841 | 0 | LEU | 105 | 42.334 | 34.703 | 52.404 | 1.00 17.74 | AAAA |
| ATOM | 842 | N | ALA | 106 | 40.532 | 34.531 | 51.095 | 1.00 19.28 | AAAA |
| ATOM | 843 | CA | ALA | 106 | 39.601 | 34.493 | 52.224 | 1.00 12.55 | AAAA |
| ATOM | 844 | CB | ALA | 106 | 38.140 | 34.574 | 51.704 | 1.00 11.58 | AAAA |
| | 845 | С | ALA | 106 | 39.807 | 33.210 | 53.023 | 1.00 14.79 | AAAA |
| ATOM | 846 | ŏ | ALA | 106 | 39.704 | 33.203 | | 1.00 13.58 | AAAA |
| MOTA | 847 | N | THR | 107 | 40.114 | 32.128 | | 1.00 13.67 | AAAA |
| ATOM | 848 | CA | THR | 107 | 40.314 | 30.819 | | | AAAA |
| ATOM | 849 | CB | THR | 107 | 40.187 | 29.708 | | | AAAA |
| MOTA | | | THR | 107 | 38.868 | 29.792 | 51.334 | | - |
| ATOM | 850 | | THR | 107 | 40.422 | 28.311 | | | AAAA |
| MOTA | 851 | | THR | 107 | 41.649 | 30.751 | | 1.00 15.80 | AAAA |
| ATCM | 852 | C | | 107 | 41.734 | 30.206 | 54.792 | | AAAA |
| ATOM | 853 | O N | THR | 108 | 42.696 | 31.294 | | | AAAA |
| MOTA | 854 | N | GLY | 108 | 43.968 | 31.298 | 53.765 | | AAAA |
| ATOM | 855 | CA | GLY | 108 | 43.801 | | | 1.00 20.05 | AAAA |
| ATOM | 856 | Ċ | GLY | 108 | 44.417 | 31.813 | | 1.00 17.53 | AAAA |
| MOTA | 857 | 0 | GLY | 109 | 42.963 | 33.158 | | | AAAA |
| ATCM | 858 | N | SER | 103 | -2.503 | 22.230 | - | | • |
| | | | • | | | | | | |

Figure 16-14

| | | | • | | | | |
|------------|-------------|---------|-----------|-----------------|-----------------|------------|------|
| ATON | | SER 109 | 42.727 | 34.020 | 56 153 | 1 00 4 | |
| ATO | | ER 109 | 41.906 | | | 1.00 14.54 | AAAA |
| ATON | | ER 109 | 42.627 | 230 | | 1.00 15.58 | AAAA |
| ATOM | | ER 109 | 42.037 | | 54.809 | 1.00 16.97 | AAAA |
| ATOM | 1 863 O S | ER 109 | 42.189 | | 57.297 | 1.00 15.56 | AAAA |
| ATOM | 864 N T | HR 110 | 41.261 | | 58.487 | 1.00 17.00 | AAAA |
| ATOM | 1 865 CA T | HR 110 | 40.608 | | 56.944 | 1.00 14.37 | AAAA |
| ATOM | | HR 110 | 39.452 | | 57.957 | 1.00 12.89 | AAAA |
| ATOM | | HR 110 | 20.424 | 30.628 | 57.360 | 1.00 14.54 | AAAA |
| ATOM | | HR 110 | 38.346 | 31.519 | 57.163 | 1.00 18.11 | AAAA |
| ATOM | | HR 110 | 39.061 | 29.452 | 58.278 | 1.00 12.91 | AAAA |
| ATOM | | | 41.633 | 30.524 | 58.601 | 1.00 18.44 | AAAA |
| ATOM | | | 41.574 | 30.302 | 59.806 | 1.00 16.30 | AAAA |
| ATOM | | AL 111 | 42.584 | 30.013 | 57.816 | 1.00 15.20 | MAAA |
| ATOM | | AL 111 | 43.614 | 29.180 | 58.403 | 1.00 20.45 | AAAA |
| ATOM | | L 111 | 44.517 | 28.514 | 57.323 | 1.00 20.02 | AAAA |
| | | | 45.652 | 27.765 | 58.005 | 1.00 21.79 | AAAA |
| ATOM | 875 CG2 VA | | 43.697 | 27.537 | 56.482 | 1.00 21.79 | AAAA |
| MOTA | 876 C VA | | 44.456 | 30.075 | 59.327 | 1.00 19.07 | AAAA |
| ATOM | 877 O VA | | 44.838 | 29.672 | 60.431 | 1.00 18.21 | AAAA |
| . ATOM | 878 N GL | | 44.731 | 31.302 | | 1.00 18.65 | AAAA |
| ATOM | 879 CA GL | N 112 | 45.493 | 32.232 | 58.890 | 1.00 16.82 | AAAA |
| MOTA | 880 CB GL | | 45.751 | 33.540 | 59.719 | 1.00 20.13 | AAAA |
| ATOM | 881 CG GL | N 112 | 46.593 | 33.360 | 58.970 | 1.00 22.39 | AAAA |
| ATOM | 882 CD GL | N 112 | 46.797 | | 57.723 | 1.00 21.17 | AAAA |
| ATOM | 883 OE1 GL | N 112 | 47.772 | 34.651 | 56.982 | 1.00 24.82 | AAAA |
| MOTA | 884 NE2 GLI | | 45.866 | 35.381 | 57.219 | 1.00 25.62 | AAAA |
| ATOM | 885 C GLI | | 44.743 | 34.963 | 56.091 | 1.00 13.16 | AAAA |
| MOTA | 886 O GL | | 45.340 | 32.516 | 61.012 | 1.00 23.99 | AAAA |
| ATOM | 887 N ALA | | 43.431 | 32.593 | 62.079 | 1.00 17.94 | AAAA |
| ATOM | 888 CA ALA | | 42.653 | | 60.924 | 1.00 15.60 | AAAA |
| ATOM | 889 CB ALA | | | | 62.138 | 1.00 15.04 | AAAA |
| ATOM | 890 C ALA | | 41.191 | | 61.802 | 1.00 18.65 | AAAA |
| ATOM | 891 O ALA | | 42.807 | | 63.083 | 1.00 14.84 | AAAA |
| MOTA | 892 N ILE | | 42.941 | 31.909 | 64.296 | 1.00 21.05 | AAAA |
| ATOM | 893 CA ILE | | 42.767 | 30.550 | 62.534 | 1.00 16.45 | AAAA |
| ATOM | 894 CB ILE | | | | 63.389 : | 1.00 15.38 | AAAA |
| ATOM | 895 CG2 ILE | | 42.600 | 28.100 | 62.637 : | 1.00 15.22 | AAAA |
| ATOM | 896 CG1 ILE | | 42.888 | | 63.537 : | 1.00 15.72 | AAAA |
| ATOM | 897 CD1 ILE | | 41.110 | 28.112 | | 1.00 19.28 | AAAA |
| ATOM | . 898 C ILE | 114 | | | 61.191] | 1.00 13.43 | AAAA |
| ATOM | 899 O ILE | 114 | | 29.318 á | 53.968 1 | .00 18.02 | AAAA |
| ATOM - | 900 N GLU | 115 | | | 55.156 1 | 00 20.38 | AAAA |
| ATOM | 901 CA GLU | 115 | | | 53.144 1 | 00 15.27 | AAAA |
| ATOM | 902 CB GLU | 115 | | 29.625 <i>6</i> | 53.614 1 | .00 21.48 | AAAA |
| ATOM | 903 CG GLU | 115 | | | 2.506 1 | .00 21.76 | AAAA |
| A . OM | 904 CD GLU | | | 29.080 6 | 1.386 1 | .00 15.78 | AAAA |
| A COM | 905 OE1 GLU | 115 | | 29.648 6 | 0.211 1 | .00 20.04 | AAAA |
| ATOM | 906 OE2 GLU | 115 | 49.051 3 | 0.843 6 | 0.239 1 | .00 21.48 | AAAA |
| ATOM | 907 C GLU | 115 | 48.901 2 | 8.902 5 | 9.241 1 | .00 26.59 | AAAA |
| ATOM | 908 O GLU | 115 | 46.877 3 | 0.559 6 | 4.814 1 | .00 23.55 | AAAA |
| ATOM . | | 115 | 47.509 3 | 0.212 6 | 5.815 1 | .00 23.03 | AAAA |
| ATOM | | 116 | 46.295 3 | 1.748 6 | | .00 22.73 | AAAA |
| ATOM | | 116 | 46.367 3 | | | .00 20.54 | |
| | 911 CB GLU | 116 | 45.744 3 | 4.044 6 | | .00 18.40 | AAAA |
| MOTA | .912 CG GLU | 116 | 46.562 3 | | | .00 19.76 | AAAA |
| ATOM | 913 CD GLU | 116 | | | 4.756 1. | 00 27.24 | AAAA |
| ATOM | 914 OE1 GLU | 116 | | | | 00 18.44 | AAAA |
| ATOM | 915 GE2 GLU | 116 | 48.919 3 | 4.543 - 64 | | 00 23.17 | AAAA |
| ATOM | 916 C GLU | 116 | 45.682 3 | | | 00 25.39 | AAAA |
| MOTA | 917 O GLU | 116 | | | | | AAAA |
| MOTA | 918 N PHE | 117 | | | | 00 22.87 | AAAA |
| MOTA | 919 CA PHE | 117 | | | | 00 18.78 | AAAA |
| MOTA | 920 CB PHE | 117 | | | | 00 22.11 | AAAA |
| MOTA | 921 CG PHE | 117 | | | _ | 00 23.14 | AAAA |
| MOTA | 922 CD1 PHE | 117 | | | | 00 24.06 | AAAA |
| MOTA | 923 CD2 PHE | 117 | | | | 00 19.67 | AAAA |
| MOT | 924 CE1 PHE | 117 | | | .066 1, | 00 24.08 | AAAA |
| · - · | | · | -v.115 30 | .531 70 | .586 1. | 00 23.68 | AAAA |
| | | | | | | | |

33/263 Figure 16-15

| _ | | | | | | | | | |
|--------|------|-----|------|-----|----------|--------|---------|------------|--------|
| MOTA | 925 | CE2 | PHE | 117 | 40.799 | 28.262 | 70.156 | 1.00 24.04 | AAAA |
| | | | | | 40.078 | 29.179 | 70.915 | 1.00 19.62 | AAAA |
| MOTA | 926 | cz | PHE | 117 | | | | | |
| ATOM | 927 | С | PHE | 117 | 44.587 | 30.068 | 68.747 | 1.00 23.87 | AAAA |
| ATOM | 928 | 0 | PHE | 117 | 44.613 | 30.031 | 69.979 | 1.00 24.40 | AAAA |
| | 929 | N | LEU | 118 | 45.238 | 29.194 | 67.981 | 1.00 21.09 | AAAA |
| ATOM | | | | | | | | 1.00 20.73 | |
| MOTA | 930 | CA | LEU | 118 | 46.025 | 28.113 | 68.549 | | AAAA |
| ATOM | 931- | CB | LEU | 118 | 46.358 | 27.075 | 67.480 | 1.00 17.90 | AAAA |
| | 932 | CG | LEU | 118 | 45.148 | 26.264 | 66.984 | 1.00 26.20 | AAAA |
| MOTA | | | | | | 25.288 | 65.924 | 1.00 34.23 | AAAA |
| ATOM | 933 | | LEU | 118 | 45.591 | | | | |
| ATOM | 934 | CD2 | LEU | 118 | 44.520 | 25.499 | 68.139 | 1.00 27.16 | AAAA |
| MOTA | 935 | С | LEU | 118 | - 47.290 | 28.601 | 69.238 | 1.00 26.49 | AAAA |
| | | | LEU | 118 | 47.908 | 27.856 | 69.996 | 1.00 26.34 | AAAA |
| MOTA | 936 | 0 | | | | | 68.975 | | AAAA |
| MOTA | 937 | N | LYS | 119 | 47.672 | 29.848 | | 1.00 28.92 | |
| MOTA | 938 | CA | LYS | 119 | 48.835 | 30.459 | 69.624 | 1.00 28.53 | AAAA |
| | 939 | CB | LYS | 119 | 49.392 | 31.616 | 68.805 | 1.00 30.15 | AAAA |
| ATOM | | | | | 49.915 | 31.267 | 67.437- | 1.00 35.14 | · AAAA |
| ATOM | 940 | CG | LYS | 119 | | | | | |
| ATOM | 941 | CD | LYS | 119 | 50.291 | 32.549 | 66.716 | 1.00 28.98 | AAAA |
| ATOM | 942 | CE | LYS | 119 | 50.905 | 32.262 | 65.380 | 1.00 31.07 | AAAA |
| | 943 | NZ | LYS | 119 | 51.195 | 33.551 | 64.745 | 1.00 22.46 | AAAA |
| ATOM | | | | | | 31.053 | 70.932 | 1.00 35.74 | AAAA |
| ATOM | 944 | С | LYS | 119 | 48.335 | | | | |
| ATOM | 945 | 0 | LYS | 119 | 49.117 | 31.541 | 71.750 | 1.00 27.10 | AAAA |
| MOTA | 946 | N | GLY | 120 | 47.018 | 31.050 | 71.103 | 1.00 25.20 | AAAA |
| | 947 | CA | GLY | 120 | 46.445 | 31,605 | 72.309 | 1.00 30.18 | AAAA |
| MOTA | | | | | | 33.007 | 72.122 | 1.00 31.91 | AAAA |
| ATOM | 948 | С | GLY | 120 | 45.913 | | | | |
| MOTA | 949 | 0 | GLY | 120 | 45.540 | 33.665 | 73.094 | 1.00 34.76 | AAAA |
| ATOM | 950 | N | ASN | 121 | 45.889 | 33.495 | 70.887 | 1.00 20.56 | AAAA |
| | 951 | CA | ASN | 121 | 45.353 | 34.825 | 70.681 | 1.00 25.58 | AAAA . |
| MOTA | | | | | 46.278 | 35.634 | 69.785 | 1.00 29.99 | AAAA |
| ATOM | 952 | CB | ASN | 121 | | | | | AAAA |
| ATOM | 953 | CG | asn | 121 | 47.641 | 35.827 | 70.427 | 1.00 24.43 | |
| ATOM - | 954 | OD1 | ASN | 121 | 48.396 | 34.874 | 70.588 | 1.00 54.63 | AAAA |
| ATOM | 955 | ND2 | ASN | 121 | 47.944 | 37.045 | 70.817 | 1.00 41.69 | AAAA |
| | | | ASN | 121 | 43.941 | 34.759 | 70.135 | 1.00 18.85 | AAAA |
| MOTA | 956 | C | | | | 33.675 | 69.899 | 1.00 24.77 | AAAA |
| MOTA | 957 | 0 | ASN | 121 | 43.421 | | | | |
| ATOM | 958 | N. | VAL | 122 | 43.310 | 35.918 | 69.991 | 1.00 19.55 | AAAA |
| ATOM | 959 | CA | VAL | 122 | 41.936 | 35.994 | 69.499 | 1.00 22.90 | AAAA |
| ATOM | 960 | CB | VAL | 122 | 41.053 | 36.832 | 70.449 | 1.00 31.47 | AAAA |
| | | | VAL | 122 | 39.649 | 37.006 | 69.851 | 1.00 31.52 | AAAA |
| ATOM | 961 | | | | | | 71.810 | 1.00 32.50 | AAAA |
| ATOM | 962 | CG2 | VAL | 122 | 40.986 | 36.154 | | | |
| MOTA | 963 | С | VAL | 122 | 41.953 | 36.632 | 68.130 | 1.00 16.87 | AAAA |
| ATOM | 964 | 0 | VAL | 122 | 42.518 | 37.710 | 67.938 | 1.00 24.08 | AAAA |
| | 965 | N | ALA | 123 | 41.321 | 35.983 | 67.159 | 1.00 18.67 | AAAA |
| MOTA | | | | | 41.360 | 36.532 | 65.821 | 1.00 10.18 | AAAA |
| ATOM | 966 | CA | ALA | 123 | | | | | AAAA |
| ATOM | 967 | CB | ALA | 123 | 42.346 | 35.743 | 64.990 | 1.00 19.04 | |
| ATOM | 968 | С | ALA | 123 | 40.000 | 36.551 | 65.131 | 1.00 13.72 | AAAA |
| ATOM | 969 | 0 | ALA | 123 | 39.108 | 35.761 | 65.439 | 1.00 20.78 | AAAA |
| | | | | 124 | 39.871 | 37.457 | 64.18C | 1.00 12.92 | AAAA |
| ATOM | 970 | N | PHE | | | | | 1.00 14.67 | AAAA |
| ATOM | 971 | CA | PHE | 124 | 38.649 | 37.610 | 63.401 | | AAAA |
| ATOM | 972 | CB | PHE | 124 | 37.904 | 38.878 | 63.85€ | 1.00 14.67 | |
| ATOM | 973 | CG | PHE | 124 | 36.660 | 39.209 | 63.049 | 1.00 20.28 | AAAA |
| | 974 | | PHE | 124 | 35.811 | 38.209 | 62.587 | 1.00 18.56 | AAAA |
| ATOM | - | | | | | | 62.843 | 1.00 19.53 | AAAA |
| ATOM | 975 | | PHE | 124 | 36.286 | 40.545 | | | |
| ATOM | 976 | CE1 | PHE | 124 | 34.609 | 38.532 | 61.937 | 1.00 18.75 | AAAA |
| ATOM | 977 | CE2 | | 124 | 35.072 | 40.875 | 62.193 | 1.00 20.18 | AAAA |
| | | CZ | PHE | 124 | 34.242 | 39.867 | 61.744 | 1.00 21.57 | AAAA |
| MOTA | 978 | | | | | 37.712 | 61.930 | 1.00 22.60 | AAAA |
| MOTA | 979 | С | PHE | 124 | 39.016 | | | | AAAA |
| ATOM | 980 | 0 | PHE | 124 | 39.823 | 38.558 | 61.535 | 1.00 19.22 | |
| ATOM | 981 | N | ASN | 125 | 38.449 | 36.820 | 61.126 | 1.00 19.39 | AAAA |
| | 982 | CA | ASN | 125 | 38.651 | 36.858 | 59.691 | 1.00 16.80 | AAAA |
| ATOM | | | | | | 35.507 | 59.150 | 1.00 15.71 | AAAA |
| ATOM | 983 | CB | ASN | 125 | 39.122 | | | | AAAA |
| ATCM | 984 | CG | ASN | 125 | 39.063 | 35.469 | 57.649 | 1.00 12.84 | |
| ATOM | 985 | OD1 | | 125 | 39.216 | 36.508 | 57.006 | 1.00 14.91 | AAAA. |
| | | ND2 | | 125 | 38.853 | 34.272 | 57.065 | 1.00 16.21 | AAAA |
| ATOM | 986 | | | | 37.315 | 37.210 | 59.038 | 1.00 16.22 | AAAA |
| ATCM | 987 | C | ASN | 125 | | | | | AAAA |
| ATOM | 988 | 0 | ASN | 125 | 36.502 | 36.330 | 58.755 | 1.00 15.28 | |
| ATOM | 989 | N | PRO | 126 | 37.071 | 38.502 | 58.775 | 1.00 14.84 | AAAA |
| • | 990 | CD | PRO | 126 | 37.908 | 39.684 | 59.052 | 1.00 18.10 | AAAA |
| atom | 990 | ٠. | 11.0 | | | | - | | • |
| • | | | | | | | | • | |

| ATO: | M 991 | CA | PRO | 126 | 3 = 4 | | | | |
|--------|---------|-------|------------|-----|--------|----------|-----------|--------------|--------|
| | | | | 126 | 35.8 | 11 38.9; | 10 58.15 | 6 1.00 17.3 | 3 аааа |
| OTA | | CB | PRO | 126 | 35.9 | 12 40.43 | 34 58.17 | 7 1.00 16.3 | |
| ATO | M 993 | CG | PRO | 126 | 37.4 | | | | |
| ATO | M · 994 | С | PRO | 126 | 35.54 | | | | |
| ATO | | ŏ | | | _ | | | | аааа 8 |
| | | | PRO | 126 | 34.40 | 04 38.29 | 91 56.32 | 2 1.00 17.0 | |
| ATO | | Ŋ | ALA | 127 | 36.60 | 7 37.97 | 72 56.043 | | |
| ATO | M 997 | CA | ALA | 127 | 36.46 | | | | |
| ATON | y 998 | CB | ALA | 127 | | | | | |
| ATON | | | | | 37.81 | | | 0 1.00 14.48 | в алла |
| | | С | ALA | 127 | 35.98 | | 8 54.702 | 2 1.00 19.7 | |
| ATON | 1 1000 | 0 | ALA | 127 | 35.49 | 0 35.50 | | | |
| ATOM | 1 1001 | N | GLY | 128 | 36.11 | | | | |
| ATOM | | CA | GLY | | | | | | 4 AAAA |
| | | | | 128 | 35.72 | 5 33.93 | 9 55.971 | 1.00 13.53 | 3 AAAA |
| ATOM | | С | GLY | 128 | 34.23 | 4 33.67 | 9 56.101 | | |
| MOTA | 1 1004 | 0 | GLY | 128 | 33.41 | | | | |
| ATOM | 1 1005 | N | GLY | 129 | | | | | АААА 🤅 |
| ATOM | | | | | 33.88 | | | 1.00 13.35 | AAAA 🤄 |
| | | CA | GLY | 129 | 32.48 | 7 32.05 | 8 56.446 | | |
| ATOM | 1007 | С | GLY | 129 | 31.75 | 4 31.83 | | | |
| ATOM | 1008 | 0 | GLY | 129 | 30.54 | | | | |
| ATOM | | N | MET | | | | | |) AAAA |
| | | | | 130 | 32.47 | | 8 54.079 | 1.00 15.00 | AAAA |
| ATOM | | CA | MET | 130 | 31.87 | 9 31.16 | 3 52.757 | 1.00 13.35 | |
| ATOM | 1011 | CB | MET | 130 | 32.96 | | | | |
| MOTA | 1012 | CG | MET | 130 | 33.68 | | | | AAAA |
| ATOM | | | | | | | | | AAAA |
| | | | MET | 130 | 34.863 | 32.87 | 7 50.425 | 1.00 15.41 | AAAA |
| MOTA | | CE | MET | 130 | 33.752 | 32.97 | 3 49.073 | | |
| ATOM | 1015 | С | MET | 130 | 31.296 | | | | |
| ATOM | 1016 | 0 | MET | 130 | 31.785 | | | | |
| ATOM | | | HÌS | | | | | 1.00 19.54 | AAAA |
| | | | | 131 | 30.188 | 29.69 | 53.617 | 1.00 16.24 | AAAA |
| MOTA | | | HIS | 131 | 29.556 | 28.448 | 3 54.014 | 1.00 13.80 | |
| ATOM | 1019 | CB . | HIS | 131 | 28.772 | | | | |
| ATOM | 1020 | CG : | HIS | 131 | 27.606 | | | 1.00 15.91 | |
| ATOM | 1021 | CD2 | | | | | _ | 1.00 13.08 | |
| | | | | 131 | 26.712 | | 56.096 | 1.00 12.46 | AAAA |
| ATOM | 1022 | ND1 | | 131 | 27.225 | 30.190 | 53.976 | 1.00 22.48 | |
| MOTA | 1023 | CE1 1 | HIS | 131 | 26.148 | | | 1.00 16.56 | |
| ATOM | 1024 | NE2 | HIS | 131 | 25.817 | | | 1.00 10.56 | AAAA |
| ATOM | | | HIS | | | | | 1.00 23.56 | AAAA |
| | | | | 131 | 28.673 | | 53.066 | 1.00 13.69 | AAAA |
| ATOM | | | HIS | 131 | 28.125 | 26.658 | 53.470 | 1.00 17.21 | AAAA |
| MOTA | 1027 | n f | HIS | 132 | 28.523 | | | | |
| ATOM | 1028 | CA E | iis | 132 | 27.669 | | | 1.00 14.51 | AAAA |
| ATOM | | | iis | | | | | 1.00 20.19 | AAAA |
| | | | | 132 | 26.863 | 28.416 | 50.054 | 1.00 17.26 | AAAA |
| ATOM | | | IIS | 132 | 25.748 | 29.070 | 50.810 | 1.00 16.85 | AAAA |
| MOTA | 1031 | CD2 H | IIS | 132 | 24.787 | 28.542 | | 1.00 13.74 | |
| ATOM | 1032 | ND1 H | IIS | 132 | 25.497 | 30.424 | | | AAAA |
| ATOM | | CE1 H | | 132 | | | | 1.00 24.80 | AAAA |
| ATOM | | | | | 24.429 | 30.700 | 51.486 | 1.00 12.68 | AAAA |
| | | Æ2 H | | 132 | 23.980 | 29.576 | 52.010 | 1.00 28.65 | AAAA |
| ATOM | | H | IS | 132 | 28.372 | 26.412 | 49.946 | 1.00 16.89 | |
| ATOM | 1036 |) н | IS | 132 | 27.731 | 25.487 | | | AAAA |
| ATOM | 1037 | יב ו | LA | 133 | 29.669 | 25.407 | 49.460 | 1.00 14.58 | AAAA |
| ATOM | | | | | | 26.580 | 49.689 | 1.00 16.79 | AAAA |
| | | | | 133 | 30.338 | 25.680 | 48.740 | 1.00 13.76 | AAAA |
| ATOM | | B A | LA | 133 | 31.738 | 26.194 | 48.412 | 1.00 14.95 | |
| ATOM | 1040 0 | : Al | LA | 133 | 30.418 | 24.219 | | | AAAA |
| ATOM | 1041 0 | | | | | | 49.179 | 1.00 18.80 | AAAA |
| | _ | | | | 30.557 | 23.939 | 50355 | 1.00 16.86 | AAAA |
| MOTA | | | | 134 | 30.306 | 23.306 | 48.209 | 1.00 13.76 | AAAA |
| MOTA | 1043 C | A PI | !Ε | 134 | 30.378 | 21.868 | 48.451 | 1.00 19.77 | |
| ATOM | 1044 C | B PF | IE : | 134 | 29.311 | 21.132 | | | AAAA |
| ATOM | 1045 3 | | | | | | 47.620 | 1.00 15.59 | AAAA |
| | | | | 134 | 27.917 | 21.525 | 47.975 | 1.00 17.22 | AAAA |
| ATOM | | D1 PH | | 134 | 27.135 | 22.259 | 47.091 | 1.00 17.88 | AAAA |
| MOTA | 1047 0 | D2 PH | E j | L34 | 27.392 | 21.187 | 49.222 | | |
| MOTA | | E1 PH | | .34 | 25.836 | | | 1.00 21.68 | AAAA |
| ATOM | | E2 PH | | | | 22.653 | 47.445 | 1.00 23.07 | AAAA |
| | | | | 134 | 26.099 | 21.578 | 49.585 | 1.00 17.64 | AAAA |
| ATCM | 1050 32 | Z PH | E] | .34 | 25.323 | 22.308 | 48.696 | 1.00 19.71 | AAAA |
| MOTA | 1051 c | PH | E 1 | .34 | 31.763 | 21.354 | 48.098 | _ | |
| ATOM | 1052 5 | PH | | 34 | 32.547 | | | 1.00 14.76 | AAAA |
| | | | | | | 22.049 | 47.442 | 1.00 18.05 | aaaa |
| ATOM | 1053 | LY | | .35 | 32.060 | 20.124 | 48.515 | 1.00 16.37 | AAAA |
| ATOM | בס 1054 | LY: | S 1 | 35 | 33.369 | 19.551 | 48.269 | 1.00 16.24 | |
| MOTA | 1055 CB | LY: | S 1 | 35 | 33.360 | 18.070 | | | AAAA |
| ATOM | 1056 CG | | | 35 | | | 48.699 | 1.00 21.29 | AAAA |
| A I OH | 1000 66 | L LIX | <i>-</i> 1 | د د | 34.640 | 17.300 | 48.400 | 1.00 30.43 | AAAA |
| | | • | | | | | - | | • |

Figure 16-17

| MOM | 1057 | CD | LYS | 135 | 34.597 | 15.867 | 48.977 | 1.00 30.26 | AAAA |
|--------------|--------------|--------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM ATOM | 1058 | CE | LYS | 135 | 34.862 | 15.805 | 50.486 | 1.00 35.01 | AAAA |
| ATOM | 1059 | NZ | LYS | 135 | 36.304 | 16.023 | 50.895 | 1.00 20.61 | AAAA |
| ATOM | 1060 | C | LYS | 135 | 33.854 | 19.687 | 46.836 | 1.00 16.60 | AAAA |
| ATOM | 1061 | ō | LYS | 135 | 35.020 | 20.020 | 46.584 | 1.00 17.24 | AAAA |
| ATOM | 1062 | N | SER | 136 | 32.944 | 19.483 | 45.893 | 1.00 18.01 | AAAA |
| MOTA | 1063 | CA | SER | 136 | 33.301 | 19.528 | 44.490 | 1.00 15.26 | AAAA |
| ATOM | 1064 | CB | SER | 136 | 33.339 | 18.094 | 43.940 | 1.00 18.07 | AAAA |
| ATOM | 1065 | OG | SER | 136 | 34.135 | 17.261 | 44.762 | 1.00 22.22 | AAAA |
| MOTA | 1066 | c | SER | 136 | 32.345 | 20.355 | 43.658 | 1.00 15.40 | AAAA |
| ATOM | 1067 | 0 | SER | 136 | 32.162 | 20.071 | 42.475 | 1.00 18.77 | AAAA |
| MOTA | 1068 | N | ARG | 137 | 31.754 | 21.401 | 44.237 | 1.00 19.71 | AAAA |
| ATOM | 1069 | CA | ARG | 137 | 30.805 | 22.216 | 43.482 | 1.00 17.29 | AAAA . |
| ATOM | 1070 | CB | ARG | 137 | 29.481 | 21.448 | 43.366 | 1.00 24.19 | AAAA |
| ATOM | 1071 | CG | ARG | 137 | 28.290 | 22.273 | 42.937 | 1.00 32.56 | AAAA |
| ATOM | 1072 | CD | ARG | 137 | 27.026 | 21.424 | 42.980 | 1.00 47.98 | AAAA |
| ATOM | 1073 | NE | ARG | 137 | 26.951 | 20.493 | | 1.00 50.95 | AAAA |
| ATOM | 1074 | CZ | ARG | 137 | 26.392 | 20.781 | 40.691 | 1.00 50.38 | AAAA |
| ATOM | 1075 | NH1 | ARG | 137 | 25.854 | 21.976 | 40.485 | 1.00 45.26 | AAAA |
| ATOM | 1076 | NH2 | ARG | 137 | 26.375 | 19.876 | 39.722 | 1.00 55.31 | AAAA |
| ATOM | 1077 | С | ARG | 137 | 30.537 | 23.595 | 44.095 | 1.00 16.14 | AAAA |
| MOTA | 1078 | 0 | ARG | 137 | 30.439 | 23.711 | 45.308 | 1.00 16.88 | AAAA |
| MOTA | 1079 | N | ALA | 138 | 30.395 | 24.621 | 43.252 | 1.00 18.07 1.00 21.48 | AAAA AAAA |
| MOTA | 1080 | CA | ALA | 138 | 30.117 | 25.976 | 43.735 | 1.00 21.48 | AAAA |
| MOTA | 1081 | CB | ALA | 138 | 30.460 | 27.024 | 42.631 | 1.00 21.04 | AAAA |
| MOTA | 1082 | С | ALA | 138 | 28.642 | 26.090 | 44.135 43.641 | 1.00 21.04 | AAAA |
| MOTA | 1083 | 0 | ALA | 138 | 27.798 | 25.339 | 45.029 | 1.00 13.83 | AAAA |
| ATOM | 1084 | N | ASN | 139 | 28.321 | 27.019 27.158 | 45.468 | 1.00 13.03 | AAAA |
| MOTA | 1085 | CA | ASN | 139 | 26.952 | 25.899 | 46.274 | 1.00 13.14 | AAAA |
| MOTA | 1086 | CB | ASN | 139 | 26.566 25.162 | 25.961 | 46.832 | 1.00 20.34 | AAAA |
| MOTA | 1087 | CG | ASN | 139 | 24.186 | 26.068 | 46.086 | 1.00 19.76 | AAAA |
| MOTA | 1088 | | ASN | 139 139 | 25.048 | | 48.157 | 1.00 16.36 | AAAA |
| ATOM | 1089 | | ASN | 139 | 26.756 | 28.409 | 46.315 | 1.00 20.92 | AAAA |
| ATOM | 1090 | C | asn asn | 139 | 27.603 | 28.738 | 47.148 | 1.00 16.81 | AAAA |
| MOTA | 1091 1092 | N O | GLY | 140 | 25.644 | 29.105 | 46.086 | 1.00 19.30 | AAAA |
| MOTA | 1092 | CA | GLY | 140 | 25.330 | 30.295 | 46.864 | 1.00 21.34 | AAAA |
| ATOM | 1094 | C | GLY | 140 | 26.393 | 31.378 | 46.888 | 1.00 20.19 | AAAA |
| ATOM ATOM | 1095 | Ö | GLY | 140 | 26.653 | 31.968 | 47.943 | 1.00 18.77 | AAAA |
| MOTA | 1096 | N | PHE | 141 | 26.996 | 31.649 | 45.733 | 1.00 15.52 | AAAA |
| MOTA | 1097 | CA | PHE | 141 | 28.034 | 32.675 | 45.600 | 1.00 20.71 | AAAA |
| ATOM | 1098 | CB | PHE | 141 | 27.711 | 33.952 | 46.388 | 1.00 20.03 | AAAA |
| ATOM | 1099 | CG | PHE | 141 | 26.355 | 34.544 | 46.127 | 1.00 28.32 | AAAA |
| MOTA | 1100 | | PHE | 141 | 25.855 | 35.526 | 46.997 | 1.00 24.25 | AAAA |
| ATOM | 1101 | CD2 | PHE | 141 | 25.589 | 34.170 | 45.029 | 1.00 30.11 | AAAA AAAA |
| ATOM | 1102 | CE1 | PHE | 141 | 24.628 | 36.116 | 46.775 | 1.00 25.94 | AAAA |
| ATOM | 1103 | CE2 | PHE | 141 | 24.346 | 34.766 | 44.801 | 1.00 21.6: 1.00 24.4 | AAAA |
| ATOM | 1104 | CZ | PHE | 141 | 23.870 | 35.741 | 45.677 | 1.00 14.45 | AAAA |
| ATOM | 1105 | С | PHE | 141 | 29.357 | 32.188 | 46.158 | 1.00 16.39 | AAAA |
| ATOM | 1106 | 0 | PHE | 141 | 30.336 | 32.914 | 46.111 46.716 | 1.00 16.77 | AAAA |
| ATOM | 1107 | N | CYS | 142 | 29.389 | 30.982 | 47.285 | 1.00 17.71 | AAAA |
| ATOM | 1108 | | CYS | 142 | 30.629 30.347 | 30.466 29.845 | 48.659 | 1.00 13.95 | AAAA |
| MOTA | 1109 | CB | CYS | 142 | | 30.985 | 49.846 | 1.00 16.63 | AAAA |
| ATOM | 1110 | SG | CYS | 142 | 29.606 31.313 | 29.421 | 46.401 | 1.00 18.09 | AAAA |
| MOTA | 1111 | C | CYS | 142 | 30.647 | 28.527 | 45.856 | | AAAA |
| MOTA | 1112 | 0 | CYS | 142 | | 29.539 | 46.272 | 1.00 12.50 | AAAA |
| MOTA | 1113 | N | TYR | 143 | 32.639 33.429 | 28.603 | 45.478 | 1.00 15.32 | AAAA |
| MOTA | 1114 | CA | TYR | 143 | 34.333 | 29.322 | 44.473 | 1.00 13.07 | AAAA |
| ATOM | 1115 | CB | TYR | 143 | 33.614 | 30.338 | 43.612 | 1.00 15.80 | AAAA |
| MOTA | 1116 | CG | TYR | 143 143 | 33.396 | 31.636 | 44.071 | 1.00 15.48 | AAAA |
| ATOM | 1117 | | TYR | 143 | 32.740 | 32.589 | 43.270 | 1.00 11.99 | AAAA |
| ATOM | 1118 | | TYR | 143 | 33.157 | 29.999 | 42.336 | 1.00 14.60 | AAAA |
| ATOM | 1119 | | TYR TYR | 143 | 32.501 | 30.935 | 41.532 | 1.00 10.74 | AAAA |
| MOTA | 1120 | CZ | TYR | 143 | 32.301 | 32.229 | 42.008 | 1.00 20.89 | AAAA |
| ATOM | 1121 1122 | OH | TYR | 143 | 31.698 | 33.177 | 41.208 | 1.00 18.87 | AAAA |
| MOTA | 1146 | | . 1,1 | | | | - | | • |
| | | | | | | | | | |

| MOTA | | _ : _ | | | 34.31 | .0 27.72 | 23 46.35 | 8 1.00 17.35 | |
|--------------|--------------|---------|------------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| 4OTA | | | | | 34.58 | 1 26.57 | | | |
| ATOM | | | | | 34.76 | | | | AAA AAA |
| MOTA MOTA | | | A ILE | | 35.59 | | | B 1.00 14.17 | AAA |
| ATOM | | | B ILE G2 ILE | | 37.01 | | | | AAAA |
| ATOM | | | G1 ILE | | 37.86 | _ | | | AAA |
| ATOM | | _ | D1 ILE | | 37.61 39.05 | | | | AAA |
| ATOM | | | | | 34.95 | | | | AAAA |
| ATOM | | | | | 34.60 | | | | AAAA |
| ATOM | | | ASN | 145 | 34.79 | | | | . AAAA |
| ATOM | | | | | 34.17 | | | | AAAA |
| MOTA | | | | | 33.40 | 1 25.17 | 8 51.988 | | AAAA AAAA |
| MOTA MOTA | | | 3 ASN D1 ASN | | 32.42 | | | 1.00 15:64 | AAAA |
| ATOM | | | DI ASN D2 ASN | | 22.00 | | - | 1.00 14.97 | AAAA |
| ATOM | | | ASN ASN | | 31.17 | | | | AAAA |
| ATOM | | _ | ASN | 145 | 35.260 35.812 | | | | AAAA |
| ATOM | 114 | 1 N | ASN | 146 | 35.599 | 27.86 | | | AAAA |
| ATOM | | | ASN | 146 | 36.685 | | | | AAAA |
| MOTA | 114 | | | 146 | 37.161 | 29.46 | | | AAAA |
| ATOM | 1144 | | | 146 | 36.101 | 30.39 | 54.865 | | AAAA AAAA |
| MOTA MOTA | 1149 1148 | | 1 ASN | 146 | 50.445 | | 7 56.034 | | AAAA |
| ATOM | 1147 | | 2 ASN ASN | 146 146 | 35.156 | | | | AAAA |
| MOTA | 1148 | | ASN | 146 | 36.306 37.160 | | | 1.00 13.04 | AAAA |
| ATOM | 1149 | | PRO | 147 | 35.025 | | | 1.00 14.76 | AAAA |
| ATOM | 1150 | CD (| | 147 | 33.817 | | | 1.00 14.28 | AAAA |
| ATOM | 1151 | | PRO | 147 | 34.750 | 26.843 | | 1.00 7.62 1.00 13.51 | AAAA |
| MOTA | 1152 | | PRO | 147 | 33.251 | 27.058 | | 1.00 14.44 | AAAA AAAA |
| MOTA MOTA | 1153 1154 | | PRO | 147 | 33.056 | | | 1.00 12.32 | AAAA |
| ATOM | 1155 | | PRO PRO | 147 147 | 35.118 | 25.330 | | 1.00 18.86 | AAAA |
| ATOM | 1156 | | ALA | 148 | 35.678 34.818 | 24.796 | | 1.00 16.24 | AAAA |
| ATOM | 1157 | | ALA | 148 | 35.122 | 24.642 23.200 | | 1.00 15.01 | AAAA |
| ATOM | 1158 | | ALA | 148 | 34.402 | 22.561 | | 1.00 15.58 1.00 12.93 | AAAA |
| ATOM | 1159 | | ALA | 148 | 36.624 | 22.956 | | 1.00 14.94 | AAAA AAAA |
| MOTA MOTA | 1160 | 0 | ALA | 148 | 37.138 | 21.999 | 56.560 | 1.00 14.69 | AAAA |
| ATOM | 1161 1162 | N CA | VAL VAL | 149 | 37.328 | 23.817 | | 1.00 12.49 | AAAA |
| MOTA | 1163 | CB | VAL | 149 149 | 38.778 39.364 | 23.708 | | 1.00 15.31 | AAAA |
| ATOM | 1164 | | VAL | 149 | 40.899 | 24.797 24.870 | 54.243 | 1.00 14.77 | AAAA |
| MOTA | 1165 | | VAL | 149 | 38.981 | 24.501 | 54.369 52.808 | 1.00 14.68 | AAAA |
| ATOM | 1166 | C | VAL | 149 | 39.323 | 23.887 | 56.572 | 1.00 12.50 1.00 20.14 | AAAA |
| ATOM | 1167 | 0 | VAL | 149 | 40.172 | 23.109 | 57.028 | 1.00 17.32 | AAAA AAAA |
| MOTA MOTA | 1168 | N | GLY | 150 | 38.815 | 24.899 | 57.271 | 1.00 15.45 | AAAA |
| ATOM | 1169 1170 | CA C | GLY GLY | 50 -50 | 39.284 | 25.168 | 58.622 | 1.00 20.96 | AAAA |
| ATOM | 1171 | Ö | GLY | 150 | 39.030 39.888 | 24.053 | 59.621 | 1.00 24.16 | AAAA |
| ATOM | 1172 | N | ILE | 151 | 37.842 | 23.738 23.465 | 60.458 | 1.00 19.50 | AAAA |
| ATOM | 1173 | CA | ILE | 151 | 37.490 | 22.375 | 59.557 60.461 | 1.00 16.67 | AAAA |
| MOTA | 1174 | CB | ILE | 151 | 35.992 | 22.052 | 60.348 | 1.00 19.56 1.00 16.46 | AAAA |
| ATOM | 1175 | CG2 | | 151 | 35.667 | 20.709 | 61.036 | 1.00 17.93 | AAAA AAAA |
| MOTA | 1176 | CG1 | | 151 | 35.180 | 23.209 | 60.959 | 1.00 12.31 | AAAA |
| MOTA MOTA | 1177 1178 | CDI | | 151 | 33.686 | 23.123 | 60.672 | 1.00 18.71 | AAAA |
| ATOM | 1179 | С 0 | ILE | 151 | 38.352 | 21.148 | 60.164 | 1.00 22.66 | AAAA |
| ATOM | 1180 | | GLU | 151 152 | 38.796 38.599 | 20.472 | 61.087 | 1.00 20.08 | AAAA |
| ATOM | 1181 | | GLU | 152 | 39.434 | 20.861 19.718 | 58.888 | 1.00 19.71 | AAAA |
| ATOM | 1182 | | GLU | 152 | 39.362 | 19.437 | 58.533 57.033 | 1.00 13.85 1.00 20.21 | AAAA |
| ATOM | 1183 | CG . | GLU | 152 | 38.033 | 18.833 | 56.624 | 1.00 20.21 | AAAA AAAA |
| ATOM | 1184 | | GLU | 152 | 37.838 | 17.430 | 57.166 | 1.00 26.94 | AAAA AAAA |
| ATOM | 1185 | OE1 | GLU | 152 | 36.720 | 16.906 | 57.035 | 1.00 25.03 | AAAA |
| atom atom | 1186 1187 | ĆE2 | | 152 | 38.800 | 16.846 | 57.708 | 1.00 24.95 | AAAA |
| atom Atom | 1188 | | | 152 152 | 40.865 | 20.010 | 58.942 | 1.00 16.85 | AAAA |
| | | | <i>ع</i> لاق | 176 | 41.629 | 19.110 | 59.289 | 1.00 19.25 | AAAA |
| | | | | | | | | | |

| | | | | | | | 21 200 | 58.931 | 1.00 | 14.74 | AAAA |
|-------|------|-----|-------|-------------|------|-------|--------|----------------|------|---------|--------|
| MOTA | 1189 | N | TYR | 153 | | 228 | 21.290 | 59.350 | 1.00 | | AAAA |
| ATOM | 1190 | CA | TYR | 153 | 42. | 574 | 21.672 | | 1.00 | 12 26 | AAAA |
| MOTA | 1191 | CB | TYR | 153 | 42. | 757 | 23.193 | 59.179 | | | AAAA |
| MOTA | 1192 | CG | TYR | · 153 | 44. | 059 | 23.727 | 59.729 | 1.00 | 10.30 | |
| | 1193 | | TYR | 153 | 45. | 234 | 23.726 | 58.967 | 1.00 | | AAAA |
| MOTA | 1194 | | TYR | 153 | 46. | 438 | 24.219 | 59.511 | 1.00 | | AAAA |
| MOTA | _ | | TYR | 153 | | 115 | 24.220 | 61.028 | 1.00 | | AAAA |
| MOTA | 1195 | | | 153 | | 288 | 24.705 | 61.570 | 1.00 | 19.76 | AAAA |
| MOTA | 1196 | | TYR | | | 440 | 24.711 | 60.824 | 1.00 | 25.97 | AAAA |
| MOTA | 1197 | CZ | TYR | 153 | | 571 | 25.235 | 61.410 | 1.00 | 23.15 | AAAA |
| ATOM | 1198 | OH | TYR | 153 | | | 21.274 | 60.828 | 1.00 | | AAAA |
| MOTA | 1199 | С | TYR | 153 | | 712 | 20.698 | 61.247 | 1.00 | | AAAA |
| MOTA | 1200 | 0 | TYR | 153 | | 722 | | 61.616 | 3 00 | 17.78 | AAAA ` |
| ATOM | 1201 | N | LEU | 154 | | 683 | 21.569 | 63.042 | 1 00 | 17.26 | AAAA |
| ATOM | 1202 | CA | LEU | 154 | | 698 | 21.239 | | 1 00 | 20.44 | AAAA |
| MOTA | 1203 | CB | LEU | 154 | | .511 | 21.913 | 63.744 | | 19.57 | AAAA |
| ATOM | 1204 | CG | LEU. | 154 | 40 | 636 | 23.434 | 63.942 | | | AAAA |
| | 1205 | | LEU | 154 | 39 | . 277 | 24.046 | 64.309 | | 22.48 | |
| MOTA | 1205 | | LEU | 154 | 41 | 692 | 23.709 | 65.044 | | 20.84 | AAAA |
| MOTA | | C | LEU | 154 | 41 | 669 | 19.715 | 63.262 | | 19.69 | AAAA |
| MOTA | 1207 | Ö | LEU | 154 | | .357 | 19.191 | 64.149 | | 22.91 | AAAA |
| MOTA | 1208 | | | 155 | | .878 | 18.996 | 62.469 | | 20.88 | AAAA |
| MOTA | 1209 | N | ARG | 155 | | .840 | 17.539 | 62.622 | 1.00 | 22.64 | AAAA |
| MOTA | 1210 | CA | ARG | | | .829 | 16.905 | 61.652 | 1.00 | 25.69 | AAAA |
| MOTA | 1211 | CB | ARG | 155 | | .384 | 17.394 | 61.893 | 1.00 | 27.64 | AAAA |
| MOTA | 1212 | CG | ARG | 155 | | .382 | 16.834 | 60.892 | 1.00 | 25.67 | AAAA |
| MOTA | 1213 | CD | ARG | 155 | | | 15.497 | 61.246 | 1.00 | 30.88 | AAAA |
| MOTA | 1214 | NE | ARG | 155 | | .931 | 14.753 | 60.488 | 1.00 | 36.28 | AAAA |
| MOTA | 1215 | cz | ARG | 155 | | .135 | 15.218 | 59.318 | 1 00 | 26.96 | AAAA |
| MOTA | 1216 | NH1 | ARG | 155 | | .705 | | 60.923 | 1 00 | 27.33 | AAAA |
| ATOM | 1217 | NH2 | ARG | 155 | | .737 | 13.562 | 62.390 | 1 00 | 28.00 | AAAA |
| MOTA | 1218 | С | ARG | 155 | | .235 | 16.966 | | 1 00 | 28.05 | AAAA |
| MOTA | 1219 | 0 | ARG · | 155 | | .674 | 16.070 | 63.119 | 1.00 | 23.53 | AAAA |
| MOTA | 1220 | N | LYS | 156 | | .949 | 17.486 | 61.395 | 1.00 | 26.79 | AAAA |
| MOTA | 1221 | CA | LYS | 156 | 44 | .290 | 16.977 | 61.128 | 1.00 | 20.73 | AAAA |
| | 1222 | ÇВ | LYS | 156 | 44 | .854 | 17.558 | 59.824 | 1.00 | 26.01 | AAAA |
| MOTA | 1223 | CG | LYS | 156 | 46 | :213 | 16.955 | 59.444 | 1.00 | 29.70 | AAAA |
| MOTA | 1224 | CD | LYS | 156 | 46 | .632 | 17.308 | 58.035 | 1.00 | 28.77 | AAAA |
| ATOM | 1225 | CE | LYS | 156 | 45 | . 685 | 16.692 | 5 7.005 | 1.00 | 39.79 | AAAA |
| MOTA | 1226 | NZ | LYS | 156 | | .671 | 15.192 | 57.058 | | 36.33 | AAAA |
| ATOM | | C | LYS | 156 | 45 | .233 | 17.260 | 62.299 | 1.00 | 26.40 | |
| MOTA | 1227 | 0 | LYS | 156 | | .188 | 16.511 | 62.529 | 1.00 | 26.19 | AAAA |
| ATOM | 1228 | | LYS | 157 | . 44 | .960 | 18.337 | 63.032 | 1.00 | 22.50 | AAAA |
| MOTA | 1229 | N | | 157 | | .757 | 18.709 | 64.204 | 1.00 | 21.12 | AAAA |
| MOTA | 1230 | CA | LYS | 157 | | .535 | 20.181 | 64.591 | 1.00 | 28.95 | AAAA |
| MOTA | 1231 | CB | LYS | | | .160 | 21.215 | | 1.00 | 25.94 | AAAA |
| MOTA | 1232 | CG | LYS | 157 | | .669 | 21.067 | | 1.00 | 35.16 | AAAA |
| ATOM | 1233 | CD | LYS | 157 | | .281 | 22.099 | | 1.00 | 39.24 | AAAA |
| MOTA | 1234 | CE | LYS | 157 | | .742 | 21.869 | | 1.00 | 40.01 | AAAA |
| ATCM | 1235 | NZ | LYS | 15 7 | | | 17.825 | | 1.00 | 22.98 | AAAA |
| MOTA | 1236 | С | LYS | 157 | | .421 | 17.903 | | 1.00 | 27.77 | AAAA |
| ATCM | 1237 | 0 | LYS | 157 | | .085 | 16.995 | | 1 00 | 26.49 | AAAA |
| ATCM | 1238 | N | GLY | 158 | | 1.392 | - | | 1 00 | 24.82 | AAAA |
| ATOM | 1239 | CA | GLY | | | 1.023 | 16.106 | | 1.00 | 33.13 | AAAA |
| ATCM | 1240 | С | GLY | 158 | | 2.771 | 16.459 | | 1.00 | 27.21 | AAAA |
| MOTA | 1241 | 0 | GLY | 158 | | 2.421 | 15.775 | 68.128 | | 27.47 | AAAA |
| ATOM | 1242 | N | PHE | 159 | | 2.085 | 17.529 | | | 24.15 | AAAA |
| | 1243 | CA | PHE | 159 | 4 (| 0.866 | | | | 0 29.12 | AAAA |
| MOTA | 1244 | CB | PHE | 159 | | .410 | | | | 27.53 | AAAA |
| MOTA | 1245 | CG | PHE | 159 | 4 | 1.264 | 20.343 | | 1.00 | 0 27.26 | AAAA |
| ATOM | | | 1 PHE | 159 | | 2.439 | | 67.220 | 1.0 | 0 28.12 | |
| ATOM | 1246 | | 2 PHE | 159 | | 926 | | 69.076 | 1.0 | 0 21.10 | AAAA |
| MOTA | 1247 | | | 159 | | 3.264 | | | 1.0 | 0 26.24 | AAAA |
| ATCM | 1248 | | 1 PHE | 159 | | 1.738 | | | 1.0 | 0 26.07 | AAAA |
| ATOM | 1249 | | | | | 2.907 | | | 1.0 | 0 23.91 | · AAAA |
| ATCM | 1250 | | | 159 | | 9.792 | | | 1.0 | 0 28.02 | AAAA |
| ATOM | 1251 | | PHE | 159 | | | | · | 1.0 | 0 21.14 | AAAA |
| ATCM | 1252 | 0 | PHE | 159 | | 9.639 | | | 1.0 | 0 24.79 | AAAA |
| ATCM | 1253 | N | LYS | 160 | | 9.056 | | | | 0 24.26 | AAAA |
| ETOM: | 1254 | | LYS | 160 | 3 | 8.011 | 15.366 | . 01.001 | | | • |

| ATO: | | | LYS | 160 | 31 | 8.360 | 14.09 | 8 68.66 | 0 1 0 | | |
|--------------|--------------|--------|------------|------------|--------------|------------|------------------|------------------|--------|--------------------|--------------|
| ATO | | | LYS | 160 | | 9.625 | | | | 0 22.86 0 43.16 | AAA |
| ATO | | | LYS | 160 | | 222 | | | 1 1 0 | 0 54.05 | AAA |
| ATO | | | LYS | 160 | 39 | 236 | 11.34 | | | 0 62.87 | AAA |
| ATO | | _ | LYS | 160 | 38 | 3.154 | 11.89 | | | 0 68.11 | AAA |
| ATO | | - | LYS | 160 | 36 | .599 | 15.82 | | | 0 21.12 | AAAA |
| ATON | | | LYS | 160 | | .632 | 15.67 | 2 68.05 | | 0 22.43 | AAA |
| ATOM | | | ARG | 161 | | .476 | 17.042 | 2 68.73 | | 0 19.68 | AAA. |
| ATON | | | ARG | .161 | 35 | .164 | 17.59 | | | 0 20.84 | AAAA |
| ATOM | | | ARG | 161 | 34 | .865 | 17.467 | 7 70.57 | | 0 26.02 | AAAA |
| ATOM ATOM | | | ARG | 161 | | .715 | 16.031 | | | 0 28.47 | AAAA |
| ATOM | | | ARG | . 161 | | .213 | 16.025 | | | 0 30.38 | AAAA AAAA |
| ATOM | | | ARG | 161 | | .098 | 16.734 | | | 0 32.99 | AAAA AAAA |
| MOTA | | | ARG | 161 | | .272 | 16.278 | | 1.0 | 0 40.49 | AAAA |
| ATOM | | | ARG ARG | 161 | | .724 | 15.094 | 73.489 | 1.0 | 31.49 | AAAA |
| ATOM | | C | | 161 | | .003 | 17.014 | 74.712 | | 38.54 | AAAA - |
| ATOM | | o | ARG ARG | 161 | | .171 | 19.060 | 68.680 | 1.00 | 18.98 | AAAA |
| ATOM | | N | | 161 | 35 | . 552 | 19.932 | | 1.00 | 23.57 | AAAA |
| MOTA | | CA | ILE ILE | 162 | | 743 | 19.332 | | 1.00 | 19.82 | AAAA |
| ATOM | | CB | ILE | 162 | | 744 | 20.700 | | 1.00 | 17.81 | AAAA |
| ATOM | | CG2 | TLE | 162 | | 522 | 20.717 | | 1.00 | 18.33 | AAAA |
| ATOM | | CG1 | THE | 162 162 | | 542 | 22.110 | | 1.00 | 13.65 | AAAA |
| ATOM | 1278 | CD1 | | 162 | 36. | 937 | 20.200 | | 1.00 | 18.15 | AAAA |
| ATOM | 1279 | C | ILE | 162 | | 722 | 19.852 | 64.670 | 1.00 | 22.52 | AAAA |
| ATOM | | ō | ILE | 162 | | 316 520 | 21.184 | 66.724 | 1.00 | 14.71 | AAAA |
| ATOM | 1281 | | LEU | 163 | | 996 | 20.492 | 66.126 | 1.00 | 17.99 | AAAA |
| ATOM | 1282 | | LEU | 163 | | 653 | 22.374 | 67.217 | 1.00 | 16.93 | AAAA |
| ATOM | 1283 | | LEU | 163 | 31. | | 22.902 23.376 | 67:061 | 1.00 | 20.73. | AAAA |
| MOTA | 1284 | CG | LEU | 163 | 29. | | 24.236 | 68.421 | 1.00 | 18.45 | AAAA |
| MOTA | 1285 | CD1 | LEU | 163 | 28. | | 23.408 | 68.463 67.975 | | 19.99 | AAAA |
| ATOM | 1286 | CD2 | LEU | 163 | 29. | | 24.751 | 69.870 | 1.00 | 15.66 | AAAA |
| MOTA | 1287 | C ; | LEU | 163 | 31. | 705 | 24.071 | 66.106 | 1.00 | 18.74 | AAAA |
| MOTA | 1288 | 0 1 | LEU | 163 | 32. | | 24.889 | 66.188 | 1.00 | 18.40 18.65 | AAAA |
| MOTA | 1289 | | TYR | 164 | 30. | | 24.128 | 65.186 | 1.00 | 18.65 | AAAA |
| MOTA | 1290 | | ΓΥR | 164 | 30.6 | | 25.246 | 64.252 | 1 00 | 11.76 | AAAA |
| ATOM | 1291 | | ryr | 164 | 30.7 | | 24.754 | 62.816 | 1.00 | 14.07 | AAAA AAAA |
| ATOM ATOM | 1292 1293 | | ryr | 164 | 30.5 | | 25.851 | 61.797 | 1.00 | 14.51 | AAAA |
| ATOM | 1293 | CD1 7 | LXK | 164 | 31.5 | | 26.822 | 61.562 | 1.00 | 27.08 | AAAA |
| ATOM | 1295 | CD2 T | TH. | 164 | 31.3 | | 27.832 | 60.598 | 1.00 | 26.21 | AAAA |
| ATOM | 1296 | CE2 T | | 164 | 29.4 | | 25.916 | 61.070 | 1.00 | 21.45 | AAAA |
| ATOM | | | YR | 164 164 | 29.1 | | 26.891 | 60.137 | 1.00 | 21.89 | AAAA |
| ATOM | | | | 164 | 30.1 | | 27.839 | 59.896 | 1.00 | 16.35 | AAAA |
| ATOM | | | | 164 | 29.8 | | 28.764 | 58.913 | 1.00 | 27.44 | AAAA |
| MOTA | | | | 164 | 29.2 28.1 | | 25.873 | 64.463 | 1.00 | 15.67 | AAAA |
| ATOM - | | | | 165 | 29 | | 25.177 | 64.455 | 1.00 | 16.07 | AAAA |
| ATOM | 1302 | | | 165 | 27.: | | 27.187 27.887 | 64.674 | 1.00 | 14.52 | AAAA |
| MOTA | 1303. | | | 165 | 27.9 | | .7.887 !8.596 | 64.893 | 1.00 | 18.37 | AAAA |
| MOTA | 1304 (| CG2 II | | 165 | 26.6 | | 9.359 | 66.254 | 1.00 | 13.31 | AAAA |
| ATOM | | CG1 II | | 165 | 28.1 | - | 7.573 | 66.419 | 1.00 | 13.06 | AAAA |
| MOTA | | D1 II | LE] | 165 | 28.49 | | 8.209 | 67.376 68.739 | 1.00 | | AAAA |
| ATOM | 1307 (| | | 165 | 27.85 | | 8.926 | 63.779 | 1.00 | | AAAA |
| MOTA | 1308 | | .E] | 65 | 28.75 | 59 2 | | 63.569 | 1.00 | | AAAA |
| ATOM | 1309 N | | | .66 | 26.72 | | 8.901 | 63.084 | 1.00 | | AAAA |
| ATOM | | A AS | P 1 | .66 | 26.50 | _ | 9.779 | 61.942 | 1.00 | | AAAA |
| ATOM | | B AS | - | 66 | 26.27 | | | 60.698 | 1.00 | | AAAA |
| ATOM | | G AS | | 66 | 26.27 | 9 29 | | 59.393 | 1.00 | | AAAA |
| ATOM | 1313 0 | D1 AS | P 1 | 66 | 25.37 | 8 30 | 0.508 | 59.213 | 1.00 | | AAAA AAAA |
| ATOM | | D2 AS | | 66 | 27.18 | 7 29 | _ | 58.551 | 1.00 | | AAAA |
| MOTA | 1315 C | | | 66 | 25.33 | 4 30 | | | 1.00 | | AAAA |
| MOTA | 1316 0 | | | 66 | 24.16 | 0 30 | 0.355 | 62.137 | 1.00 | | AAAA |
| MOTA | 1317 N | | | 67 | 25.64 | | 2.010 | 62.407 | 1.00 | | AAAA |
| TOM TOM | 1318 C | | | 67 | 24.59 | | 2.993 | 62.665 | 1.00 | | AAAA |
| | 1319 ÇI | | | 67 67 | 25.05 | 1 33 | 3.962 i | 63.767 | 1.00 1 | | AAAA |
| 1107 | 1320 C | LE | J 10 | 5 7 | 25.34 | 5.33 | .239 | | 1.00 1 | | AAAA |
| | | • | | | | | - | • | | | |

| | | | | | • | | | | |
|-------|------|-----|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 1321 | CD1 | LEU | 167 | 25.635 | 34.271 | 66.169 | 1.00 28.82 | AAAA |
| ATOM | 1322 | CD2 | | 167 | 24.148 | 32.372 | 65.513 | 1.00 18.59 | AAAA |
| ATOM | 1323 | С | LEU | 167 | 24.122 | 33.776 | 61.449 | 1.00 12.62 | AAAA |
| MOTA | 1324 | 0 | LEU | 167 | 23.288 | 34.678 | 61.570 | 1.00 15.00 | AAAA |
| ATOM | 1325 | N | ASP | 168 | 24.667 | 33.431 | 60.288 | 1.00 14.35 | AAAA |
| ATOM | 1326 | CA | ASP | 168 | 24.277 | 34.056 | 59.022 | 1.00 19.50 | AAAA |
| MOTA | 1327 | CB | ASP | 168 | 25.060 | 33.409 | 57.880 | 1.00 25.15 | AAAA |
| ATOM | 1328 | CG | ASP | 168 | 24.908 | 34.145 | 56.573 | 1.00 48.45 | AAAA |
| ATOM | 1329 | OD1 | ASP | 168 | 25.477 | 35.247 | 56.454 | 1.00 64.45 | AAAA |
| ATOM | 1330 | OD2 | ASP | 168 | 24.215 | 33.633 | 55.668 | 1.00 44.71 | AAAA |
| MOTA | 1331 | С | ASP | 168 | 22.787 | 33.751 | 58.834 | 1.00 16:30 | AAAA |
| MOTA | 1332 | 0 | ASP | 168 | 22.327 | 32.696 | 59.252 | 1.00 17.72 | AAAA |
| ATOM | 1333 | N | ALA | 169 | 22.059 | 34.657 | 58.175 | 1.00 14.11 | AAAA . |
| 'ATOM | 1334 | CA | ALA | 169 | 20.618 | 34.503 | 57.934 | 1.00 19.61 | AAAA . |
| MOTA | 1335 | CB | ALA | 169 | 20.006 | 35.856 | 57.470 | 1.00 13.56 | AAAA |
| ATOM | 1336 | С | ALA | 169 | 20.277 | 33.400 | 56.926 | 1.00 18.23 | AAAA |
| ATOM | 1337 | 0 | ALA | 169 | 19.105 | 33.159 | 56.641 | 1.00 17.20 | AAAA |
| ATOM | 1338 | N | HIS | 170 | 21.301 | 32.750 | 56.373 | 1.00 16.53 | AAAA |
| MOTA | 1339 | CA | HIS | 170 | 21.075 | 31.652 | 55.436 | 1.00 17.51 | AAAA |
| ATOM | 1340 | CB | HIS | 170 | 21.616 | 31.973 | 54.033 | 1.00 22.32 | AAAA |
| ATOM | 1341 | CG | HIS | 170 | 20.954 | 33.142 | 53.377 | 1.00 25.38 | AAAA |
| ATOM | 1342 | CD2 | HIS | 170 | 19.934 | 33.196 | 52.487 | 1.00 19.33 | AAAA AAAA |
| ATOM | 1343 | ND1 | HIS | 170 | 21.308 | 34.448 | 53.638 | 1.00 18.17 | AAAA |
| ATOM | 1344 | CE1 | HIS | 170 | 20.535 | 35.257 | 52.935 | 1.00 30.34 | AAAA |
| ATOM | 1345 | NE2 | HIS | 170 | 19.692 | 34.523 | 52.229 | 1.00 17.51 | AAAA . |
| ATOM | 1346 | С | HIS | 170 | 21.781 | 30.413 | 55.967 | 1.00 16.72 1.00 15.92 | AAAA |
| ATOM | 1347 | 0 | HIS | 170 | 22.827 | 30.511 | 56.610 | 1.00 15.28 | ÁAAA |
| ATOM | 1348 | N | HIS | 171 | 21.209 | 29.245 | 55.682 | 1.00 15.28 | AAAA |
| MOTA | 1349 | CA | HIS | 171 | 21.751 | 27.961 | 56.123 | 1.00 12.33 | AAAA |
| MOTA | 1350 | CB | HIS | 171 | 20.702 | 26.878 | 55.814 | 1.00 17.27 | AAAA |
| MOTA | 1351 | CG | HIS | 171 | 21.180 | 25.468 | 55.980 | 1.00 17.27 | AAAA |
| MOTA | 1352 | CD2 | HIS | 171 | 21.249 | 24.447 | 55.090 | 1.00 26.73 | AAAA |
| MOTA | 1353 | | HIS | 171 | 21.622 | 24.956 | 57.181 57.021 | 1.00 15.98 | AAAA |
| MOTA | 1354 | | HIS | 171 | 21.948 | 23.685 | 55.761 | 1.00 20.03 | AAAA |
| ATOM | 1355 | | HIS | 171 | 21.729 | 23.352 | 55.498 | 1.00 15.55 | AAAA |
| MOTA | 1356 | С | HIS | 171 | 23.107 | 27.602 27.784 | 54.298 | 1.00 17.03 | AAAA |
| MOTA | 1357 | 0 | HIS | 171 | 23.318 | 27.105 | 56.323 | 1.00 14.33 | AAAA |
| MOTA | 1358 | N | CYS | 172 | 24.026 25.350 | 26.675 | 55.866 | 1.00 13.65 | AAAA |
| ATOM | 1359 | CA | CYS | 172 | 26.330 | 26.631 | 57.054 | 1.00 12.99 | AAAA |
| MOTA | 1360 | CB | CYS | 172 | 25.680 | 25.826 | 58.551 | 1.00 17.17 | AAAA |
| MOTA | 1361 | SG | CYS | 172 | 25.212 | 25.274 | 55.257 | 1.00 16.52 | AAAA |
| MOTA | 1362 | C | CYS | 172 | 25.750 | 24.297 | 55.783 | 1.00 14.95 | AAAA |
| ATOM | 1363 | 0 | CYS | 172 173 | 24.516 | 25.173 | 54.130 | 1.00 15.42 | AAAA |
| ATOM | 1364 | N | ASP | 173 | 24.302 | 23.865 | 53.531 | 1.00 14.75 | AAAA |
| MOTA | 1365 | CA | ASP | 173 | 23.339 | 23.956 | 52.332 | 1.00 17.73 | AAAA |
| ATOM | 1366 | CB | ASP ASP | 173 | 23.765 | 24.966 | 51.283 | 1.00 22.84 | AAAA |
| MOTA | 1367 | CG | ASP | 173 | 23.106 | 24.998 | 50.216 | 1.00 18.68 | AAAA |
| MOTA | 1368 | | ASP | 173 | 24.730 | 25.728 | 51.504 | 1.00 15.34 | AAAA |
| MOTA | 1369 | C | ASP | 173 | 25.590 | 23.145 | 53.149 | 1.00 16.39 | AAAA |
| ATOM | 1370 | Ö | ASP | 173 | 25.684 | 21.922 | 53.279 | 1.00 15.48 | AAAA |
| ATOM | 1371 | Ŋ | GLY | 174 | 26.583 | 23.912 | 52.705 | 1.00 15.58 | AAAA |
| MOTA | 1372 | CA | GLY | 174 | 27.869 | 23.346 | 52.360 | 1.00 13.97 | AAAA |
| MOTA | 1373 | C | GLY | 174 | 28.508 | 22.723 | 53.595 | 1.00 18.44 | AAAA |
| MOTA | 1374 | ō | GLY | 174 | 28.970 | 21.586 | 53.540 | 1.00 15.48 | AAAA |
| ATOM | 1375 | N | VAL | 175 | 28.554 | 23.456 | 54.706 | 1.00 16.84 | AAAA |
| ATOM | 1376 | CA | AYP | 175 | 29.136 | 22.923 | 55.946 | 1.00 16.54 | AAAA |
| ATOM | 1377 | CB | AYL | 175 | 29.201 | 24.031 | 57.037 | 1.00 15.88 | AAAA |
| MOTA | 1378 | | VAL | 175 | 29.927 | 23.507 | 58.307 | 1.00 15.35 | AAAA |
| ATOM | 1379 | | VAL | 175 | 29.923 | 25.258 | 56.476 | 1.00 15.62 | AAAA |
| ATOM | 1380 | CGZ | VAL | 175 | 28.318 | 21.720 | 56.467 | 1.00 19.21 | AAAA |
| ATOM | 1381 | 0 | VAL | 175 | 28.876 | 20.735 | 56.961 | 1.00 17.75 | AAAA |
| ATOM | 1382 | N | GLN | 176 | 26.996 | 21.798 | 56.367 | 1.00 17.74 | AAAA |
| ATOM | 1383 | CA | GLN | 176 | 26.164 | 20.685 | | 1.00 15.66 | AAAA |
| MOTA | 1384 | CB | GLN | 176 | 24.678 | 20.973 | 56.595 | 1.00 16.64 | AAAA |
| ATOM | 1385 | CG | GLN | 176 | 23.789 | 19.788 | 56.952 | | AAAA |
| MOTA | 1386 | | ٧٠٠٠٠ | | | | - | | • |
| | | | | _ | | | | | |

| MOTA | 138 | | _ | | 22.325 | 20.106 | 56.884 | 1.00 21.52 | AAAA |
|--------------|--------------|----------|----------------|--------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1388 | | E1 GLN | | 21.850 | | | | AAAA |
| MOTA | 1389 | | E2 GLN | | 21.581 | | | | AAAA |
| ATOM ATOM | 1390 1391 | | GLN GLN | | 26.527 | | | | AAAA |
| ATOM | 1392 | | GLU | | 26.751 26.581 | | | | AAAA |
| ATOM | 1393 | | | | 26.909 | | | | AAAA |
| ATOM | 1394 | | | | 26.857 | | | | AAAA |
| MOTA | 1395 | | | 177 | 27.131 | | | | AAAA |
| ATOM | 1396 | CE | | 177 | 26.960 | | | | AAAA AAAA |
| MOTA | 1397 | | 1 GLU | 177 | 27.974 | 17.935 | | | AAAA |
| MOTA | 1398 | | | 177 | 25.796 | 17.853 | | 1.00 26.89 | AAAA |
| MOTA | 1399 | | GLU | . 177 | 28.284 | | 54.376 | 1.00 20.42 | AAAA |
| MOTA | 1400 1401 | | GLU | 177 | 28.486 | | 54.527 | 1.00 17.05 | AAAA |
| MOTA MOTA | 1401 | | ALA ALA | 178 178 | 29.233 30.611 | | 54.527 | 1.00 19.67 | AAAA |
| MOTA | 1403 | | | 178 | 31.464 | | 54.839 | 1.00 18.18 | AAAA |
| MOTA | 1404 | | ALA | 178 | 30.806 | 17.418 | 54.918 56.106 | 1.00 12.76 1.00 17.56 | AAAA |
| ATOM | 1405 | | ALA | 178 | 31.690 | 16.555 | 56.167 | 1.00 17.30 | AAAA AAAA |
| ATOM | 1406 | Ŋ | PHE | 179 | 29.981 | 17.656 | 57.116 | 1.00 18.82 | AAAA |
| MOTA | 1407 | CA | PHE | 179 | 30.124 | 16.945 | 58.379 | 1.00 20.26 | AAAA |
| MOTA | 1408 | CB | PHE | 179 | 30.554 | 17.948 | 59.439 | 1.00 13.17 | AAAA |
| ATOM | 1409 | CG | PHE | 179 | 31.779 | 18.693 | 59.048 | 1.00 16.28 | AAAA |
| MOTA MOTA | 1410 1411 | | 1 PHE 2 PHE | 179 179 | 31.705 | 20.017 | 58.610 | 1.00 13.77 | AAAA |
| ATOM | 1412 | | 1 PHE | 179 | 33.002 32.845 | 18.031 20.673 | 58.995 | 1.00 15.57 | AAAA |
| ATOM | 1413 | | 2 PHE | 179 | 34.145 | 18.677 | 58.114 58.500 | 1.00 20.03 1.00 20.30 | AAAA |
| ATOM | 1414 | CZ | PHE | 179 | 34.060 | 20.002 | 58.058 | 1.00 20.50 | AAAA AAAA |
| MOTA | 1415 | С | PHE | 179 | 28.882 | 16.219 | 58.833 | 1.00 18.52 | AAAA |
| MOTA | 1416 | 0 | PHE | 179 | 28.773 | 15.828 | 60.000 | 1.00 20.21 | AAAA |
| ATOM | 1417 | N | TYR | 180 | 27.969 | 16.016 | 57.895 | 1.00 18.33 | AAAA |
| MOTA MOTA | 1418 1419 | CA CB | TYR TYR | 180 180 | 26.698 | 15.379 | 58.176 | 1.00 19.93 | AAAA |
| ATOM | 1420 | CG | TYR | 180 | 25.874 24.402 | 15.310 15.341 | • | 1.00 20.97 | AAAA |
| ATOM | 1421 | | TYR | 180 | 23.565 | 14.337 | 57.159 56.686 | 1.00 19.80 1.00 23.87 | AAAA AAAA |
| ATOM | 1422 | , | TYR | 180 | 22.203 | 14.391 | 56.898 | 1.00 21.32 | AAAA |
| MOTA | 1423 | | TYR | 180 | 23.831 | 16.416 | 57.865 | 1.00 19.02 | AAAA |
| ATOM | 1424 | CE2 | | 180 | 22.470 | 16.482 | 58.084 | 1.00 26.84 | AAAA |
| ATOM | 1425 | CZ | TYR | 180 | 21.659 | 15.462 | 57.594 | 1.00 30.54 | AAAA |
| MOTA MOTA | 1426 1427 | C OH | TYR TYR | · 180 180 | 20.310 | 15.514 | 57.794 | 1.00 22.81 | AAAA |
| ATOM | 1428 | ō | TYR | 180 | 26.855 26.064 | 13.970 13.526 | 58.737 59.579 | 1.00 22.61 | AAAA |
| ATOM | 1429 | N | ASP | 181 | 27.893 | 13.328 | 58.253 | 1.00 23.44 1.00 22.27 | AAAA AAAA |
| ATOM | 1430 | CA | ASP | 181 | 28.245 | 11.920 | 58.590 | 1.00 33.84 | AAAA |
| MOTA | 1431 | CB | ASP | 181 | 28.916 | 11.318 | 57.339 | 1.00 41.74 | AAAA |
| MOTA | 1432 | CG | ASP | 181 | 30.035 | 10.363 | 57.662 | 1.00 57.71 | AAAA |
| MOTA | 1433 1434 | | ASP | 181 | 30.999 | 10.780 | 58.340 | 1.00 61.40 | AAAA |
| MOTA MOTA | 1435 | C | ASP ASP | 181 181 | 29.965 29.107 | 9.197 | 57.221 | 1.00 65.77 | AAAA |
| ATOM | 1436 | ō | ASP | 181 | 29.307 | 11.654 10.497 | 59.838 60.227 | 1.00 30.21 1.00 27.84 | AAAA |
| ATOM | 1437 | N | THR | 182 | 29.615 | 12.696 | | 1.00 27.53 | AAAA AAAA |
| ATOM | 1438 | CA | THR | 182 | 30.472 | 12.466 | 61.634 | 1.00 21.19 | AAAA |
| ATOM | 1439 | CB | THR | 182 | 31.918 | 12.977 | 61.358 | 1.00 26.55 | AAAA |
| MOTA | 1440 | | | 182 | 32.729 | 12.763 | 62.513 | 1.00 25.62 | AAAA |
| ATOM | 1441 | | | 182 | 31.922 | 14.471 | 61.037 | 1.00 21.67 | AAAA |
| ATOM | 1442 | C | THR | 182 | 30.010 | 13.050 | 62.954 | 1.00 25.02 | AAAA |
| MOTA MOTA | 1443 1444 | O N | THR ASP | 182 183 | 29.306 30.434 | 14.049 | 62.992 | 1.00 23.56 | AAAA |
| ATOM | 1445 | | ASP | 183 | 30.086 | 12.424 12.894 | 64.042 65.371 | 1.00 19.66 1.00 21.52 | AAAA |
| ATOM | 1446 | СВ | ASP | 183 | 29.735 | 12.894 | 66.275 | 1.00 21.52 | AAAA AAAA |
| ATOM | 1447 | | ASP | 183 | 30.920 | 10.783 | 66.523 | 1.00 20.32 | AAAA :: |
| MOTA | 1448 | OD1 | ASP | 183 | 31.667 | 10.502 | 65.565 | 1.00 30.99 | AAAA |
| atom | | OD2 | | 183 | 31.095 | 10.326 | 67.675 | 1.00 48.65 | AAAA |
| ATOM | | | ASP | 183 | 31.257 | 13.685 | 65.947 | 1.00 16.66 | AAAA |
| ATOM | | | ASP | 183 | 31.236 | 14.092 | 67.104 | 1.00 23.37 | AAAA. |
| MOTA | 1452 | N | GLN | 184 | 32.286 | 13.909 | 65.131 | 1.00 21.95 | AAAA |

SUBSTITUTE SHEET (RULE 26)

Figure 16-23

| | | ~3 | OT N | 304 | 33.437 | 14.672 | 65.590 | 1.00 17.65 | AAAA |
|----------|-------------|-----|-------|-------|--------|--------|--------|------------|--------|
| MOTA | 1453 | CA | GLN | 184 | | | 64.866 | 1.00 21.36 | AAAA |
| ATOM | 1454 | CB | GLM | 184 | 34.701 | 14.243 | | 1.00 27.38 | AAAA |
| MOTA | 1455 | CG | GLN | 184 | 35.068 | 12.790 | 65.102 | 1.00 27.38 | AAAA |
| MOTA | 1456 | CD | GLN | 184 | 36.485 | 12.476 | 64.691 | | |
| MOTA | 1457 | OE1 | GLN | 184 | 36.899 | 12.760 | 63.573 | 1.00 29.90 | AAAA |
| ATOM | 1458 | NE2 | GLN | 184 | 37.239 | 11878 | 65.599 | 1.00 31.84 | AAAA |
| ATOM | 1459 | | GLN | 184 | 33.207 | 16.165 | 65.382 | 1.00 18.54 | AAAA |
| | 1460 | ō | GLN . | | 33.881 | 17.009 | 65.972 | 1.00 18.11 | AAAA |
| MOTA | | | VAL | 185 | 32.258 | 16.481 | 64.519 | 1.00 19.18 | AAAA |
| MOTA | 1461 | N | | | 31.934 | 17.872 | 64.267 | 1.00 21.57 | AAAA |
| MOTA | 1462 | CA | VAL | 185 | 32.261 | 18.264 | 62.807 | 1.00 22.64 | AAAA |
| ATOM | 1463 | CB | VAL | 185 - | | | 62.591 | 1.00 16.26 | AAAA |
| ATOM | 1464 | | VAL | 185 | 31.994 | 19.768 | 62.500 | 1.00 16.77 | AAAA |
| ATOM | 1465 | CG2 | VAL | 185 | 33.722 | 17.924 | | 1.00 16.77 | AAAA |
| MOTA | 1466 | С | VAL | 185 | 30.449 | 18.035 | 64.523 | | AAAA |
| MOTA | 1467 | 0 | VAL | 185 | 29.658 | 17.156 | 64.179 | 1.00 20.79 | |
| ATOM | 1468 | N | PHE . | 186 | 30.081 | 19.146 | 65.153 | 1.00 18.73 | AAAA |
| ATOM | 1469 | CA | PHE | 186 | 28.687 | 19.446 | 65.435 | 1.00 16.22 | AAAA |
| ATOM | 1470 | CB | PHE | 186 | 28.432 | 19.559 | 66.952 | 1.00 16.83 | AAAA |
| | 1471 | CG | PHE | 186 | 26.976 | 19.682 | 67.299 | 1.00 17.96 | , AAAA |
| MOTA | 1472 | | PHE | 186 | 26.319 | 18.656 | 67.968 | 1.00 23.24 | AAAA |
| ATOM | 1473 | | PHE | 186 | 26.240 | 20.797 | 66.904 | 1.00 15.41 | AAAA |
| ATOM | | | | 186 | 24.953 | 18.738 | 68.235 | 1.00 18.99 | AAAA |
| MOTA | 1474 | | PHE | | 24.879 | 20.887 | 67.168 | 1.00 24.05 | AAAA |
| MOTA | 1475 | | PHE | 186 | 24.234 | 19.846 | 67.838 | 1.00 22.93 | AAAA |
| MOTA | 1476 | CZ | PHE | 186 | | | 64.778 | 1.00 17.16 | AAAA |
| MOTA | 1477 | С | PHE | 186 | 28.437 | 20.789 | 64.993 | 1.00 19.37 | AAAA |
| MOTA | 1478 | 0 | PHE | 186 | 29.192 | 21.725 | | 1.00 19.67 | AAAA |
| MOTA | 1479 | N | VAL | 187 | 27.391 | 20.874 | 63.961 | 1.00 17.74 | AAAA |
| MOTA | 1480 | CA | VAL | 187 | 27.075 | 22.116 | 63.277 | | AAAA |
| MOTA | 1481 | CB | VAL | 187 | 27.010 | 21.914 | 61.720 | 1.00 18.65 | AAAA |
| ATOM | 1482 | CG1 | VAL | 187 | 26.578 | 23.211 | 61.024 | 1.00 17.31 | AAAA |
| ATOM | 1483 | CG2 | VAL | - 187 | 28.359 | 21.453 | 61.194 | 1.00 16.65 | |
| ATOM | 1484 | С | VAL | 187 | 25.732 | 22.637 | 63.746 | 1.00 18.46 | AAAA |
| ATOM | 1485 | Ō | VAL | 187 | 24.752 | 21.903 | 63.764 | 1.00 20.64 | AAAA |
| ATOM | 1486 | N | LEU | 188 | 25.708 | 23.899 | 64.150 | 1.00 14.42 | AAAA |
| ATOM | 1487 | CA | LEU | 188 | 24.482 | 24.563 | 64.567 | 1.00 16.68 | AAAA |
| MOTA | 1488 | CB | LEU | 188 | 24.568 | 25.070 | 66.009 | 1.00 13.98 | AAAA |
| | 1489 | CG | LEU | 188 | 23.522 | 26.119 | 66.450 | 1.00 13.66 | AAAA |
| MOTA | 1490 | | LEU | 188 | 22.103 | 25.556 | 66.401 | 1.00 15.55 | AAAA |
| MOTA | | | LEU | 188 | 23.844 | 26.585 | 67.861 | 1.00 16.40 | AAAA |
| ATOM | 1491 | | | 188 | 24.272 | 25.756 | 63.667 | 1.00 20.01 | AAAA |
| MOTA | 1492 | C | LEU | | 25.164 | 26.595 | 63.506 | 1.00 18.86 | AAAA |
| MOTA | 1493 | 0 | LEU | 188 | 23.104 | 25.845 | 63.057 | 1.00 14.46 | AAAA |
| MOTA | 1494 | Ŋ | SER | 189 | | 27.011 | 62.230 | 1.00 14.56 | AAAA |
| MOTA | 1495 | CA | SER | 189 | 22.841 | 26.668 | 60.737 | 1.00 15.55 | AAAA |
| ATOM | 1496 | CB | SER | 189 | 22.896 | | 60.008 | 1.00 14.09 | AAAA |
| ATOM | 1497 | OG | SER | 189 | 22.619 | 27.851 | | 1.00 15.24 | AAAA |
| MOTA | 1498 | С | SER | 189 | 21.487 | 27.606 | 62.508 | 1.00 21.46 | AAAA |
| MOTA | 1499 | 0 | SER | 189 | 20.509 | 26.885 | 62.578 | | AAAA |
| MOTA | 1500 | N | LEU | 190 | 21.423 | 28.921 | 62.690 | 1.00 14.92 | AAAA |
| ATOM | 1501 | CA | LEU | 190 | 20.128 | 29.572 | 62.826 | 1.00 15.54 | AAAA |
| ATOM | 1502 | CB | LEU | 190 | 20.084 | 30.663 | 63.906 | 1.00 21.02 | |
| ATOM | 1503 | CG | LEU | 190 | 20.594 | 30.532 | 65.339 | 1.00 30.17 | AAAA |
| ATOM | 1504 | | LEU | 190 | 19.736 | 31.437 | 66.210 | 1.00 19.75 | AAAA |
| | 1505 | | LEU | 190 | 20.547 | 29.130 | 65.831 | 1.00 19.08 | AAAA |
| ATOM | 1506 | c | LEU | 190 | 20.035 | 30.250 | 61.456 | 1.00 14.31 | AAAA |
| ATOM | 1507 | ō | LEU | 190 | 21.031 | 30.752 | 60.951 | 1.00 15.43 | AAAA |
| ATOM | | | | 191 | 18.855 | 30.285 | 60.856 | 1.00 16.88 | AAAA |
| ATOM | 1508 | | HIS | 191 | 18.732 | 30.884 | 59.535 | 1.00 14.34 | AAAA |
| MOTA | 1509 | CA | HIS | | 19.506 | 30.015 | 58.539 | 1.00 17.34 | AAAA |
| MOTA | 1510 | CB | HIS | 191 | 19.229 | 28.546 | 58.697 | 1.00 14.27 | AAAA |
| ATOM | 1511 | CG | HIS | 191 | | | 59.319 | 1.00 9.60 | AAAA |
| ATOM | 1512 | | HIS | 191 | 19.941 | 27.578 | 58.247 | 1.00 21.22 | AAAA |
| ATOM | 1513 | | HIS | 191 | 18.073 | 27.940 | | 1.00 21.22 | AAAA |
| ATOM | 1514 | | HIS | 191 | 18.088 | 25.660 | 58.582 | | AAAA |
| ATOM | 1515 | NE2 | HIS | 191 | 19.212 | 26.415 | 59.232 | 1.00 20.70 | AAAA |
| ATOM | 1516 | C | HIS | 191 | 17.277 | 31.026 | 59.110 | 1.00 16.19 | |
| ATOM | 1517 | ō | HIS | 191 | 16.381 | 30.489 | | 1.00 16.73 | AAAA |
| | 1518 | N | GLN | 192 | 17.044 | 31.796 | 58.045 | 1.00 14.78 | AAAA |
| ATCM . | | • | | | | | - | | • |
| | | | | | | | | | |

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Figure 16-24

| MOTA | 151 | 9 C. | GLN | 192 | 15.683 | 31.968 | 3 57.516 | 1.00 16.33 | AAAA |
|--------|--------------|----------|-------|-----|----------|--------|----------|--------------------------|-------------|
| ATOM | 152 | 0 CE | GLN | 192 | 15.669 | 32.871 | 56.283 | 1.00 17.07 | AAAA |
| ATOM | 152 | 1 CG | GLN | 192 | 16.174 | 34.270 | | 1.00 18.15 | AAAA |
| MOTA | 152 | 2 CE | GLN | 192 | 16.408 | | | 1.00 14.74 | |
| ATOM | 152 | 3 OE | 1 GLN | | 15.490 | | | 1.00 20.46 | AAAA |
| ATOM | . 1524 | | | | 17.630 | | | | AAAA |
| ATOM | 152 | | GLN | | 15.262 | | | 1.00 13.44 | AAAA |
| ATOM | 152 | | GLN | | 16.071 | | | 1.00 15.06 | AAAA |
| ATOM | 152 | | SER | | | | | 1.00 19.23 | AAAA |
| ATOM | 1528 | _ | | | 14.007 | | | 1.00 15.63 | AAAA |
| | 1529 | | _ | | 13.561 | | | 1.00 13.84 | AAAA |
| ATOM | | | _ | | 12.097 | | | 1.00 17.28 | AAAA |
| ATOM | 1530 | | SER | 193 | 11.639 | | | 1.00 17.58 | AAAA |
| ATOM | 1531 | | SER | 193 | 13.687 | | | -1.00 11.80 | AAAA |
| MOTA | 1532 | | SER | 193 | 13.400 | | 54.569 | 1.00 18.44 | AAAA |
| MOTA | 1533 | | PRO | 194 | . 14.103 | _ | 54.928 | 1.00 14.59 | AAAA |
| ATOM | 1534 | | PRO | 194 | 14.335 | 26.325 | 55.782 | 1.00 19.22 | AAAA |
| ATOM | 1535 | | PRO | 194 | 14.268 | 27.143 | 53.513 | 1.00 15.30 | AAAA |
| ATOM | 1536 | CB | PRO | 194 | 14.892 | 25.737 | 53.573 | 1.00 18.33 | AAAA |
| MOTA | 1537 | CC | PRO | 194 | 15.359 | 25.587 | 55.007 | 1.00 22.34 | AAAA |
| ATOM | 1538 | С | PRO | 194 | 12.880 | | | 1.00 16.40 | AAAA |
| MOTA | 1539 | 0 | PRO | 194 | 12.757 | 27.003 | | 1.00 19.43 | AAAA |
| ATOM | 1540 | N | GLU | 195 | 11.828 | 27.151 | | 1.00 20.57 | AAAA |
| ATOM | 1541 | CA | GLU | 195 | 10.483 | 27.161 | 53.099 | 1.00 30.15 | AAAA |
| ATOM | 1542 | CB | GLU | 195 | 9.386 | 27.037 | 54.173 | 1.00 30.13 | |
| ATOM | 1543 | | GLU | 195 | 8.987 | 28.325 | 54.879 | 1.00 45.60 | |
| ATOM | 1544 | | GLU | 195 | 7.880 | 29.119 | 54.174 | 1.00 34.45 | AAAA |
| ATOM | 1545 | | GLU | 195 | 7.635 | 30.259 | 54.612 | 1.00 43.98 | AAAA |
| ATOM | 1546 | | GLU | 195 | 7.241 | 28.627 | 53.210 | 1.00 43.98 | AAAA |
| ATOM | 1547 | c | GLU | 195 | 10.333 | 28.474 | 52.318 | | AAAA |
| ATOM | 1548 | ō | GLU | 195 | 9.522 | 28.557 | 51.395 | 1.00 26.92 1.00 24.59 | AAAA |
| MOTA | 1549 | N | TYR | 196 | 11.116 | 29.501 | 52.669 | | AAAA |
| MOTA | 1550 | CA | TYR | 196 | 11.024 | 30.753 | 51.922 | 1.00 18.16 | AAAA |
| ATOM · | 1551 | CB | TYR | 196 | 10.208 | 31.801 | 52.690 | 1.00 15.81 | AAAA |
| ATOM | 1552 | CG | TYR | 196 | 10.868 | | | 1.00 20.01 | AAAA |
| MOTA | 1553 | CD1 | | 196 | 11.779 | 32.353 | 53.932 | 1.00 19.77 | AAAA |
| ATOM | 1554 | CEI | | 196 | | 33.408 | 53.853 | 1.00 18.24 | AAAA |
| ATOM | 1555 | CD2 | | 196 | 12.407 | 33.898 | 54.988 | 1.00 18.50 | AAAA |
| ATOM | 1556 | CE2 | | 196 | 10.598 | 31.801 | 55.185 | 1.00 18.12 | AAAA |
| ATOM | 1557 | | | | 11.223 | 32.283 | 56.339 | 1.00 21.09 | AAAA |
| MOTA | 1558 | CZ OH | TYR | 196 | 12.125 | 33.326 | 56.235 | 1.00 20.39 | AAAA |
| ATOM | 1559 | | TYR | 196 | 12.759 | 33.784 | 57.367 | 1.00 16.20 | AAAA |
| | 1560 | C | TYR | 196 | 12.342 | 31.372 | 51.475 | 1.00 16.89 | AAAA |
| ATOM | | O | TYR | 196 | 12.336 | 32.347 | 50.718 | 1.00 23.08 | AAAA |
| MOTA | 1561 | N | ALA | 197 | 13.466 | 30.817 | 51.911 | 1.00 17.52 | AAAA |
| ATOM | 1562 | CA | ALA | 197 | 14.754 | | 51.512 | 1.00 20.26 | AAAA |
| ATOM | 1563 | CB | ALA | 197 | 15.315 | 32.261 | 52.659 | 1.00 20.74 | AAAA |
| ATOM | 1564 | C | ALA | 197 | 15.814 | 30.392 | 51.074 | 1.70 13.51 | AAAA |
| ATOM | 1565 | 0 | ALA | 197 | 15.787 | 29.229 | 51.457 | 1)0 19.35 | AAAA |
| ATOM | 1566 | N | PHE | 198 | 16.757 | 30.869 | 50.257 | 1. 70 18.01 | AAAA |
| ATOM | 1567 | CA | PHE | 198 | 17.861 | 30.049 | 49.782 | 1.00 17.97 | AAAA |
| MOTA | 1568 | СВ | PHE | 198 | | 30.933 | 49.119 | 1.00 20.38 | AAAA |
| ATOM | 1569 | CG | PHE | 198 | 20.094 | 30.162 | 48.545 | 1.00 23.61 | AAAA |
| ATOM | 1570 | | PHE | 198 | 20.039 | 29.660 | 47.245 | 1.00 29.71 | AAAA |
| ATOM | 1571 | CD2 | | 198 | 21.229 | 29.899 | 49.321 | 1.00 19.06 | AAAA |
| ATOM | 1572 | | PHE | 198 | 21.091 | 28.908 | 46.719 | 1.00 30.39 | AAAA |
| ATOM | 1573 | | PHE | 198 | 22.290 | 29.145 | 48.807 | 1.00 23.17 | AAAA |
| ATOM | 1574 | C3 | PHE | 198 | 22.218 | 28.646 | 47.493 | 1.00 22.74 | AAAA |
| ATOM | 1575 | С | PHE | 198 | 18.453 | 29.419 | 51.032 | 1.00 16.02 | AAAA |
| ATOM | 1576 | 0 | PHE | 198 | 18.552 | 30.073 | 52.061 | 1.00 20.95 | AAAA |
| ATOM | 1577 | М | PRO | 199 | 18.941 | 28.176 | 50.937 | 1.00 19.92 | AAAA |
| ATOM | 1578 | CD | PRO | 199 | 19.600 | 27.508 | 52.074 | 1.00 17.86 | AAAA |
| ATOM | 1579 | CA | PRO | 199 | 18.990 | 27.318 | 49.744 | 1.00 23.54 | AAAA |
| ATOM | 1580 | | PRO | 199 | 20.108 | 26.344 | 50.095 | 1.00 22.70 | AAAA |
| ATOM | 1581 | | PRO | 199 | 19.813 | 26.087 | 51.534 | 1.00 23.16 | AAAA |
| ATOM . | | | PRO | 199 | 17.710 | 26.595 | 49.312 | 1.00 30.97 | AAAA |
| ATOM | 1583 | | PRO | 199 | 17.733 | 25.855 | 48.322 | 1.00 23.25 | AAAA |
| ATOM | 1584 | | PHE | 200 | 16.621 | 26.795 | 50.054 | 1.00 20.32 | AAAA |
| | - | | | | | 24.133 | 20.034 | 1.00 20.32 | ****** |

| | | | | | • | | | | | | | |
|--------------|--------------|----------|------------|------------|----------------|-----|------------------|------------------|--------|----------------|--------------|---|
| | 1585 | CA | PHE | 200 | 15.31 | 9 2 | 26.166 | 49.752 | 1.00 2 | | AAAA | |
| MOTA | 1586 | CB | PHE | 200 | 14.84 | | | | 1.00 1 | .9.77 | AAAA | |
| ATOM ATOM | 1587 | CG | PHE | 200 . | 14.75 | | | | 1.00 1 | | AAAA | |
| ATOM | 1588 | CD1 | | 200 | 15.74 | | 28.644 | 47.346 | 1.00 1 | 0.06 | AAAA AAAA | |
| MOTA | 1589 | CD2 | | 200 | 13.65 | | | 48.519 | 1.00 1 | 3.00 | AAAA | |
| ATOM | 1590 | CE1 | PHE | 200 | 15.63 | | 30.003 | 47.042 | 1.00 2 | | AAAA | |
| ATOM | 1591 | CE2 | PHE | 200 | 13.53 | | 30.101 | 48.221 | 1.00 2 | | AAAA | |
| ATOM | 1592 | CZ | PHE | 200 | 14.52 | | 30.736 | 47.482 49.845 | 1.00 | | AAAA | |
| ATOM | 1593 | С | PHE | 200 | 15.29 | | 24.637 | 50.272 | 1.00 2 | | AAAA | |
| ATOM | 1594 | 0 | PHE | 200 | 14.30 | | 24.049 | 49.418 | 1.00 2 | | AAAA | |
| ATOM | 1595 | N | GLU | 201 | 16.38 | | 24.004 22.542 | 49.399 | 1.00 | | AAAA | |
| ATOM | 1596 | CA | GLU | 201 | 16.52 | | 22.542 | 48.284 | 1.00 | | AAAA | |
| ATOM | 1597 | CB | GLU | 201 | 17.49 | - | 22.140 | 46.881 | 1.00 | | AAAA | |
| MOTA | 1598 | CG | GLU | 201 | 17.02 | - | 22.265 | 45.848 | 1.00 | | AAAA | |
| MOTA | 1599 | CD | GLU | 201 | 18.12 18.70 | | 21.155 | 45.769 | 1.00 | | AAAA | |
| MOTA | 1600 | | GLU | 201 | 18.40 | | 23.230 | 45.111 | 1.00 | | AAAA | |
| MOTA | 1601 | | GLU | 201 | 17.00 | - | 21.891 | 50.695 | 1.00 | 23.51 | AAAA | |
| ATOM | 1602 | С | GLU | 201 | 16.84 | - | 20.689 | 50.886 | 1.00 | 23.17 | AAAA | |
| MOTA | 1603 | 0 | GLU | 201 202 | 17.63 | | 22.681 | 51.571 | 1.00 | | AAAA | |
| MOTA | 1604 | N | LYS | 202 | 18.17 | | 22.177 | 52.829 | 1.00 | | AAAA | |
| MOTA | 1605 | CA | LYS LYS | 202 | 19.60 | | 21.862 | 52.634 | 1.00 | | AAAA | |
| MOTA | 1606 | CB | LYS | 202 | 19.90 | | 20.769 | 51.611 | 1.00 | | AAAA | |
| MOTA | 1607 | CG CD | LYS | 202 | 20.9 | | 21.162 | 50.648 | 1.00 | | AAAA | |
| MOTA | 1608 1609 | CE | LYS | 202 | 21.0 | | 20.209 | 49.463 | | 55.83 | AAAA | |
| MOTA | 1610 | NZ | LYS | 202 | 22.0 | 24 | 20.662 | 48.422 | | 28.09 | AAAA | |
| MOTA | 1611 | c | LYS | 202 | 18.0 | 16 | 23.240 | 53.899 | | 17.02 | AAAA AAAA | |
| MOTA MOTA | 1612 | Ö | LYS | 202 | . 17.7 | 05 | 24.381 | 53.585 | | 20.20 | AAAA | |
| MOTA | 1613 | N | GLY | 203 | 18.2 | | 22.875 | 55.160 | | 22.94 19.38 | AAAA | |
| MOTA | 1614 | CA | GLY | 203 | 18.0 | | 23.850 | 56.223 57.128 | | 20.48 | AAAA | |
| MOTA | 1615 | С | GLY | 203 | 16.8 | | 23.564 | 58.070 | | 18.55 | AAAA | |
| MOTA | 1616 | 0 | GLY | 203 | 16.6 | | 24.312 | 56.852 | 1 00 | 15.42 | AAAA | |
| ATOM | 1617 | N | PHE | 204 | 16.1 | | 22.484 | 57.670 | | 20.73 | AAAA | |
| MOTA | 1618 | CA | PHE | 204 | 14.9 | | 22.143 21.212 | 56.903 | | 19.97 | AAAA | |
| MOTA | 1619 | CB. | PHE | 204 | 14.0 13.4 | | 21.838 | 55.667 | 1.00 | 19.63 | AAAA | |
| ATOM | 1620 | CG | PHE | 204 | 14.1 | | 21.801 | 54.459 | 1.00 | 24.96 | AAAA | |
| ATOM | 1621 | | PHE | 204 204 | 12.2 | 30 | 22.523 | 55.725 | 1.00 | 18.92 | AAAA | |
| MOTA | 1622 | | PHE | 204 | 13.6 | | 22.438 | 53.327 | | 20.66 | AAAA | |
| MOTA | 1623 | CE2 | | 204 | 11.7 | | 23.169 | 54.597 | 1.00 | 24.86 | AAAA | |
| ATOM | 1624 1625 | CZ | PHE | 204 | 12.4 | | 23.127 | 53.400 | 1.00 | 23.66 | AAAA AAAA | |
| MOTA | 1626 | C | PHE | 204 | 15.3 | | 21.513 | 59.006 | 1.00 | 18.73 | AAAA | |
| MOTA ATOM | 1627 | õ | PHE | 204 | 16.4 | 15 | 20.851 | 59.131 | 1.00 | 20.18 19.46 | AAAA | |
| ATOM | 1628 | Ŋ | LEU | 205 | 14.5 | | 21.726 | 59.994 | 1.00 | 21.09 | AAAA | |
| MOTA | 1629 | CA | LEU | 205 | 14.7 | | 21.244 | 61.356 | | 23.44 | · AAAA | |
| ATOM | 1630 | CB | LEU | 205 | 13.5 | | 21.674 | 62.233 63.693 | 1.00 | 23.23 | AAAA | |
| ATOM | 1631 | CG | LEU | 205 | 13.5 | | 21.222 | 64.445 | | 24.06 | AAAA | |
| ATOM | 1632 | CD1 | LEU | 205 | 14.7 | | 21.736 | 64.312 | 1.00 | 30.63 | AAAA | |
| ATOM | 1633 | CD2 | LEU | 205 | 12.2 | | 21.743 19.748 | 61.489 | | 23.53 | AAAA | 1 |
| MOTA | 1634 | С | LEU | 205 | 14.9 15.6 | | 19.315 | 62.381 | 1.00 | 21.28 | LAAA | 1 |
| ATOM | 1635 | 0 | LEU | 205 | 14.3 | | 18.959 | 60.591 | 1.00 | 21.59 | AAA? | |
| MOTA | 1636 | | GLU | 206 | 14.4 | | 17.502 | 60.686 | 1.00 | 27.89 | KAAA | |
| MOTA | 1637 | CA | GLU | 206 | 13.3 | | 16.816 | | 1.00 | 28.90 | AAA | |
| MOTA | 1638 | CB | GLU | 206 206 | 12.0 | | 17.615 | | 1.00 | 48.55 | LAAA | |
| Mota | 1639 | CG | GLU | 206 | 12.1 | | 18.832 | | 1.00 | 46.86 | AAA | |
| MOTA | 1640 | CD | GLU | 206 | 11.3 | | 19.769 | 59.178 | 1.00 | 21.58 | AAA | |
| MOTA | 1641 | | GLU | 206 | 13.0 | | 18.833 | 58.181 | | 63.58 | AAA AAA | |
| MOTA | 1642 | C | GLU | 206 | 15.8 | | 16.955 | | 1.00 | 22.86 | AAA | |
| MOTA | 1643 | 0 | GLU | 206 | 16.0 | 071 | 15.753 | | | 21.21 | AAA | |
| MOTA | 1644 1645 | И | GLU | 207 | 16.6 | | 17.816 | | 1.00 | 25.04 | AAA | |
| MOTA | 1646 | CA | GLU | 207 | 17.9 | 976 | 17.373 | | | 19.61 | AAA | |
| MOTA | 1647 | CB | GLU | 207 | 18.4 | | 18.322 | | | 18.44 | AAA | |
| MOTA MOTA | 1648 | CG | GLU | 207 | 17. | | 18.222 | | | 24.75 | AAA | |
| MOTA | 1649 | CD | GLU | 207 | 17. | | 19.514 | | 2 1 00 | 22.17 | AAA | |
| MOTA | 1650 | | 1 GLU | 207 | 18. | /38 | 20.182 | 55.948 | . 1.00 | | • | |
| ATOM | | | | • • | ٠. | | | | | | | |

| | | | _ | | | | | | | |
|----|------|-----------|------|------------|-------|--------|----------|-----------------------|--------------|-----------|
| | ATON | | 51 (| DE2 GL | บ 207 | 16.6 | 46 19.8 | 54 55.39 | c 1 00 4 | |
| | ATON | 4 165 | 52 (| GL. | U 207 | 18.9 | | | | AAAA |
| | ATOM | | | - | | | | | | AAAA |
| | | | | | | 19.50 | | 16 60.68 [.] | 7 1.00 18.11 | |
| | ATOM | _ | | | E 208 | 19.08 | 31 16.2 | 18 60.98 | | AAAA |
| | ATOM | 1 165 | 55 C | A IL | E 208 | 19.93 | | | | AAAA |
| | ATOM | 1 165 | 6 C | B IL | | | | | | Aaaa |
| ٠. | ATOM | | | | | 19.11 | | 52 63.400 | 3 1.00 28.84 | AAAA |
| | | | _ | G2 IL | | 19.96 | | 93 64.653 | 1.00 43.26 | |
| | ATOM | - | | Gl ILI | E 208 | 17.90 |)5 16.5¢ | 63.625 | | AAAA |
| | ATOM | 165 | 9 C | D1 ILI | .208 | 17.02 | 0 16 16 | 00.02 | | AAAA |
| | ATOM | 166 | | | | | | | | AAAA |
| | ATOM | | | | | 21.15 | | 60 61.981 | 1.00 24.74 | AAAA |
| | | _ | - | | | 21.78 | 5 14.85 | 0 62.943 | 1.00 22.68 | |
| | ATOM | | 2 N | GL | 209 | 21.51 | | | | AAAA |
| | ATOM | 166 | 3 C | A GLY | | 22.69 | | | | AAAA |
| | ATOM | | | | | | | | 1.00 20.43 | AAAA |
| | | | | GLY | | 22.34 | | 9 60.037 | 1.00 25.56 | |
| | MOTA | | | GLY | 209 | 21.16 | 5 12.44 | | 1.00 25.22 | AAAA |
| | MOTA | 166 | 6 N | GLU | 210 | 23.37 | | | | AAAA |
| | ATOM | 166 | 7 C. | | | | | | | AAAA |
| | ATOM | | | | | 23.23 | | | 1.00 25.78 | AAAA |
| | | | | - | | 23.40 | 4 10.73 | 1 57.835 | 1.00 28.27 | |
| | MOTA | 1669 | 9 CG | GLU | 210 | 23.04 | | 9 56.965 | | AAAA |
| | MOTA | 1670 |) CI | GLU | 210 | 23.17 | | | | AAAA |
| | MOTA | 1671 | | :1 .GLU | | | | | | AAAA |
| | ATOM | | | | 210 | 24.29 | | | 1.00 62.00 | AAAA |
| | | 1672 | | 2 GLU | 210 | 22.15 | 3 9.89 | 4 54.768 | 1.00 73.24 | |
| | MOTA | 1673 | C | GLU | 210 | 24.329 | | | | AAAA |
| | ATOM | 1674 | 0 | GLU | 210 | 25.447 | | 22.936 | | AAAA |
| | MOTA | 1675 | | GLY | | | | | 1.00 28.85 | AAAA |
| | ATOM | | | | 211 | 24.012 | | 1 60.121 | 1.00 27.84 | AAAA |
| | | 1676 | | | 211 | 24.991 | 7.50 | 2 60.657 | 1.00 26.25 | |
| | ATOM | 1677 | C | GLY | 211 | 25.545 | | | 1.00 20.25 | AAAA |
| | ATOM | 1678 | 0 | GLY | 211 | 24.788 | | | 1.00 27.79 | AAAA |
| | ATOM | 1679 | N | LYS | 212 | | | | 1.00 28.66 | AAAA |
| | ATOM | 1680 | | | | 26.865 | | 62.150 | 1.00 34.62 | AAAA |
| | | | _ | LAS. | 212 | 27.512 | 8.287 | 63.393 | 1.00 34.39 | |
| | ATOM | 1681 | CB | LYS | 212 | 29.029 | 8.132 | | 1.00 10.19 | AAAA |
| | ATOM | 1682 | CG | LYS | 212 | 29.505 | | _ | 1.00 40.40 | AAAA |
| | ATOM | 1683 | CD | LYS | 212 | | | | 1.00 53.97 | AAAA |
| | ATOM | 1684 | | | | 29.139 | | 64.131 | 1.00 61.93 | AAAA |
| | | | CE | LYS | 212 | 29.612 | 4.347 | 63.863 | 1.00 62.74 | |
| | MOTA | 1685 | NZ | LYS | 212 | 31.091 | 4.258 | | 1.00 70.11 | AAAA |
| | ATOM | 1686 | С | LYS | 212 | 27.181 | | | 1.00 /0.11 | AAAA |
| | ATOM | 1687 | 0 | LYS | 212 | 27.109 | | | 1.00 36.04 | AAAA |
| | ATOM | 1688 | N | GLY | | | | | 1.00 28.34 | AAAA |
| | | | | | 213 | 26.959 | 10.543 | 62.688 | 1.00 31.47 | AAAA |
| | MOTA | 1689 | CA | GLY | 213 | 26.648 | 11.948 | 62.898 | 1.00 31.68 | |
| | ATOM | 1690 | С | GLY | 213 | 25.189 | 12.291 | | | AAAA. |
| | ATOM | 1691 | 0 | GLY | 213 | 24.840 | | | 1.00 28.78 | AAAA |
| | MOTA | 1692 | N | LYS | | | 13.460 | 63.259 | 1.00 22.56 | AAAA |
| | ATOM | 1693 | | | 214 | 24.317 | 11.292 | 63.222 | 1.00 28.54 | AAAA |
| | | | CA | LYS | 214 | 22.905 | 11.585 | 63.463 | 1.00 31.11 | |
| | MOTA | 1694 | CB | LYS | 214 | 22.080 | 10.295 | 63.325 | | AAAA |
| | ATOM | 1695 | CG | LYS | 214 | 20.583 | | | 1.00 31.03 | AAAA |
| | ATOM | 1696 | CD | LYS | 214 | 20.303 | 10.461 | 63.224 | 1.00 38.15 | AAAA |
| | ATOM | 1697 | | | | 19.968 | 9.115 | 62.844 | 1.00 40.49 | AAAA |
| | | | CE | LYS | 214 | 18.490 | 9.22C | 62.537 | 1.00 48.02 | AAAA |
| | ATOM | 1698 | NZ | LYS | 214 | 17.927 | 7.924 | 62.064 | 1 00 44 00 | |
| | ATOM | 1699 | С | LYS | 214 | 22.834 | 12.160 | | 1.00 44.99 | AAAA |
| | MOTA | 1700 | 0 | LYS | 214 | | 12.100 | 64.875 | 1.00 26.90 | AAAA |
| | ATOM | 1701 | | | | 23.260 | 11.524 | 65.831 | 1.00 33.33 | AAAA |
| | | | N | GLY | 215 | 22.310 | 13.376 | 64.997 | 1.00 24.38 | |
| | MOTA | 1702 | CA | GLY | 215 | 22.230 | 14.034 | 66.230 | | AAAA |
| | ATOM | 1703 | С | GLY | 215 | 23.298 | 15.115 | | 1.00 26.03 | AAAA |
| | MOTA | 1704 | 0 | GLY | | | 13.113 | 66.447 | 1.00 27.03 | AAAA |
| | | | | | 215 | 23.352 | 15.820 | 67.458 | 1.00 23.34 | AAAA |
| | ATOM | 1705 | N | TYR | 216 | 24.152 | 15.260 | 65.439 | 1.00 22.79 | |
| | ATOM | 1706 | CA | TYR | 216 | 25.217 | 16.257 | | | AAAA |
| | ATOM | 1707 | CB | TYR | 216 | | 10.237 | 65.512 | 1.00 25.51 | AAAA |
| | ATOM | 1708 | | | | 26.592 | 15.576 | 65.406 | 1.00 20.54 | AAAA |
| | | | | TYR | 216 | 26.900 | 14.671 | 66.581 | 1.00 26.47 | AAAA |
| | MOTA | | CD1 | | 216 | 26.221 | 13.464 | 66.757 | 1.00 28.96 | |
| | ATOM | 1710 | CE1 | TYR | 216 | 26.455 | 12.660 | 67 870 | | AAAA |
| | ATOM | | CD2 | | 216 | 27.832 | | 67.872 | 1.00 33.08 | AAAA |
| | ATOM | | | | | | 15.052 | 67.552 | 1.00 24.21 | AAAA |
| | | _ | | TYR | 216 | 28.074 | 14.254 | 68.675 | 1.00 34.45 | AAAA |
| | MOTA | | | TYR | 216 | 27.378 | 13.063 | | 1.00 40.53 | |
| | ATOM | 1714 | OH ! | TYR | 216 | 27.580 | 12.291 | | 1 00 45 55 | AAAA |
| | ATOM | | | TYR | 216 | | 17 222 | 69.947 | 1.00 45.67 | AAAA |
| | | | | | - | 25.104 | 17.391 | 64.493 | 1.00 22.57 | AAAA |
| | | * 1 7 0 (| | TYR | 216 | 26.097 | 18.014 | | 1.00 19.70 | AAAA |
| | | | • | | • | | | • | | , P. TATA |
| | | | | | | | | | | |

45/263 Figure 16-27

| | | | | 017 | 23.889 | 17.635 | 64.027 | 1.00 22.88 | AAAA |
|--------|--------------|--------|------------|------------|--------|----------|---------|--------------------------|---|
| MOTA | 1717 | N | ASN | 217 | | 18.729 | 63.109 | 1.00 22.60 | AAAA |
| ATOM | 1718 | CA | ASN | 217 217 | | 18.240 | 61.671 | 1.00 16.61 | AAAA |
| ATOM | 1719 | CB | ASN | 217 | 23.233 | 19.387 | 60.695 | 1.00 17.16 | AAAA |
| MOTA | 1720 | CG | ASN | 217 | 22.098 | 19.704 | 60.307 | 1.00 20.23 | AAAA |
| MOTA | 1721 | OD1 | | | 24.320 | 20:032 | 60.309 | 1.00 12.18 | AAAA |
| MOTA | 1722 | ND2 | | 217 | 22.311 | 19.296 | 63.630 | 1.00 17.65 | AAAA |
| MOTA | 1723 | C | ASN | 217 | 21.381 | 18.550 | 63.894 | 1.00 17.63 | AAAA |
| MOTA | 1724 | 0 | ASN | 217 | 22.236 | 20.610 | 63.793 | 1.00 21.68 | AAAA |
| MOTA | 1725 | N | LEU | 218 | 21.014 | 21.197 | 64.320 | 1.00 21.20 | AAAA |
| MOTA | 1726 | CA | LEU | 218 | 21.186 | 21.547 | 65.808 | 1.00 17.73 | AAAA |
| MOTA | 1727 | CB | LEU | 218 - | 19.906 | 21.702 | 66.647 | 1.00 32.30 | AAAA |
| MOTA | 1728 | CG | LEU | 218 | 20.228 | 22.427 | 67.944 | 1.00 24.51 | AAAA |
| MOTA | 1729 | CD1 | LEU | 218 | 18.862 | 22.464 | 65.903 | 1.00 40.08 | AAAA |
| MOTA | 1730 | | LEU | 218 | 20.700 | 22.459 | 63.554 | 1.00 19.46 | AAAA |
| MOTA | 1731 | С | LEU | 218 | 21.467 | 23.425 | 63.615~ | 1.00 16.70 | AAAA |
| MOTA | 1732 | 0 | LEU | 218 | 19.590 | 22.441 | 62.824 | 1.00 15.43 | AAAA |
| MOTA | 1733 | N | ASN | 219 | 19.143 | 23.609 | 62.072 | 1.00 14.05 | AAAA |
| MOTA | 1734 | CA | ASN | 219 | 18.634 | 23.232 | 60.665 | 1.00 15.92 | AAAA |
| ATOM | 1735 | CB | ASN | 219 | 19.732 | 22.738 | 59.750 | 1.00 22.73 | AAAA |
| ATOM | 1736 | CG | ASN | 219 | 20.861 | 23.232 | 59.802 | 1.00 17.90 | AAAA |
| ATOM | 1737 | | ASN | 219 | 19.398 | 21.789 | 58.868 | 1.00 16.62 | AAAA |
| MOTA | 1738 | | ASN | 219 | 17.990 | 24.256 | 62.821 | 1.00 21.98 | AAAA |
| ATOM | 1739 | С | ASN | 219 | 17.075 | 23.569 | 63.262 | 1.00 18.65 | AAAA |
| MOTA | 1740 | 0 | ASN | 219 | 18.025 | 25.580 | 62.952 | 1.00 16.82 | AAAA |
| MOTA | 1741 | N | ILE | 220 | 16.951 | 26.298 | 63.640 | 1.00 13.22 | AAAA |
| MOTA | 1742 | CA | ILE | 220 | 17.522 | 27.115 | 64.823 | 1.00 15.70 | AAAA |
| MOTA | 1743 | CB | ILE | 220 | 16.411 | 27.912 | 65.479 | 1.00 15.18 | AAAA |
| MOTA | 1744 | | ILE | 220 | 18.246 | 26.193 | 65.823 | 1.00 19.11 | AAAA |
| MOTA | 1745 | CGI | ILE | 220 220 | 17.350 | 25.259 | 66.632 | 1.00 22.75 | . AAAA |
| ATOM - | 1746 | | ILE | 220 | 16.363 | 27.246 | 62.573 | 1.00 18.80 | AAAA |
| MOTA | 1747 | C | ILE | 220 | 16.810 | 28.386 | 62.419 | 1.00 15.52 | AAAA |
| MOTA | 1748 | 0 | ILE | 221 | 15.341 | 26.790 | 61.826 | 1.00 16.72 | AAAA |
| MOTA | 1749 | N | PRO | 221 | 14.612 | 25.518 | 61.906 | 1.00 18.83 | AAAA |
| MOTA | 1750 | CD | PRO PRO | 221 | 14.739 | 27.628 | 60.785 | 1.00 19.83 | AAAA |
| MOTA | 1751 | CA | PRO | 221 | 13.930 | 26.615 | 59.948 | 1.00 20.76 | AAAA |
| MOTA | 1752 | CB | PRO | 221 | 14.409 | 25.241 | 60.462 | 1.00 28.73 | AAAA AAAA |
| MOTA | 1753 | CG | PRO | 221 | 13.849 | 28.664 | 61.444 | 1.00 21.26 | AAAA |
| MOTA | 1754 | С 0 | PRO | 221 | 13.061 | 28.318 | 62.314 | 1.00 22.46 | AAAA |
| ATOM | 1755 | N | LEU | 222 | 13.977 | 29.926 | 61.028 | 1.00 19.70 1.00 21.62 | AAAA |
| ATOM | 1756 1757 | CA | LEU | 222 | 13.209 | 31.018 | 61.612 | | AAAA |
| ATOM | 1758 | CB | LEU | 222 | 14.163 | 31.972 | 62.319 | | AAAA |
| MOTA | 1759 | CG | LEU | 222 | 14.868 | 31.232 | | | AAAA |
| ATOM | 1760 | | 1 LEU | 222 | 16.026 | 32.072 | | | AAAA |
| MOTA | 1761 | | 2 LEU | 222 | 13.857 | | | | AAAA |
| ATOM | 1762 | c c | LEU | 222 | 12.350 | | | 0 07 | AAAA |
| ATOM | 1763 | ŏ | LEU | 222 | 12.687 | | | | AAAA |
| MOTA | 1764 | И | PRO | 223 | 11.220 | | 404 | | AAAA |
| MOTA | 1765 | | | 223 | 10.723 | | | | AAAA |
| MOTA | 1766 | CA | | 223 | 10.264 | | | | AAAA |
| MOTA | 1767 | | | 223 | 9.006 | | | | AAAA. |
| MOTA | 1768 | | | 223 | 9.608 | 33.304 | | | AAAA |
| MOTA | 1769 | | PRO | 223 | 10.606 | 34.458 | | | AAAA |
| MOTA | 1770 | | PRO | 223 | 11.525 | | | | AAAA |
| ATOM | 1771 | | LYS | 224 | 9.830 | 34.912 | | | AAAA |
| MOTA | 1772 | | | 224 | 9.975 | 36.254 | 58.200 | | AAAA |
| MOTA | 1773 | | | 224 | 9.002 | | | | AAAA |
| MOTA | | | | 224 | 9.163 | | | 10 | AAAA |
| ATOM | 1774 1775 | | | 224 | 8.109 | 35.68 | | 4 | AAAA |
| ATOM | 1776 | | | | 8.209 | | | | AAAA |
| MOTA | | | | | 7.207 | | | | AAAA |
| ATCM | | | LYS | | 9.638 | | | | AAAA |
| MOTA | | | LYS | | 8.819 | 37.03 | | 77 | AAAA |
| MOTA | | _ | GLY | | 10.239 | | | | AAAA |
| ATOM | | | | | 9.97 | | | | AAAA |
| ATOM | | - | GLY | | 10.55 | 5 .39.28 | 6 61.50 | 7 1.00 20.63 | *************************************** |
| MOTA | 1782 | | | ٠. | • | | | | |
| • | | | CI | Detter | T OHER | T /841 | Ť 001 | | |

SUBSTITUTE SHEET (RULE 26)

| ATOM | 1783 | 0 | GLY | 225 | 10.128 | 39.912 | 62.468 | 1.00 | 20.66 | AAAA |
|--------------|--------------|----------|------------|--------------|------------------|------------------|------------------|------|----------------|--------------|
| MOTA | 1784 | | LEU | | 11.540 | | 61.606 | 1.00 | 20.37 | AAAA |
| MOTA | 1785 | | LEU | | 12.154 | | 62.893 | 1.00 | 18.71 | AAAA |
| ATOM | 1786 | | LEU | | 13.354 | | 62.670 | | 13.63 | AAAA |
| ATOM | 1787 | | LEU | | 13.836 | | 63.939 | | 18.44 | AAAA |
| ATOM - | 1788 1789 | _ | LEU LEU | | 12.834 15.232 | | 64.243 | | 18.09 | AAAA |
| MOTA MOTA | 1790 | | LEU | | 12.649 | 35.844 39.309 | 63.741 63.642 | | 17.96 | AAAA |
| ATOM | 1791 | | LEU | | 13.320 | | 63.052 | | 19.84 18.13 | AAAA |
| ATOM | 1792 | | ASN | | 12.336 | 39.421 | 64.932 | | 23.30 | AAAA |
| ATOM | 1793 | CA | ASN | | 12.815 | 40.571 | 65.692 | | 20.88 | AAAA AAAA |
| ATOM | 1794 | CB | ASN | | 11.682 | 41.261 | 66.485 | | 21.73 | AAAA |
| ATOM | 1795 | CG | ASN | 227 | 11.061 | 40.368 | 67.546 | | 20.47 | AAAA |
| ATOM | 1796 | | ASN | | 11.762 | 39.736 | 68.341 | 1.00 | 23.80 | AAAA |
| ATOM | 1797 | | ASN | | 9.729 | 40.340 | 67.581 | | 21.08 | AAAA |
| ATOM | 1798 | C | ASN | | 13.950 | 40.152 | 66.612 | | 25.24 | -AAAA |
| MOTA | 1799 | 0 | ASN | 227 | 14.282 | 38.965 | 66.702 | | 18.54 | AAAA |
| MOTA ATOM | 1800 1801 | N CA | ASP ASP | 228 228 | 14.547 15.682 | 41.124 | 67.296 | | 19.41 | AAAA |
| ATOM | 1802 | CB | ASP | 228 | 16.208 | 40.844 42.141 | 68.169 68.802 | | 22.15 16.82 | AAAA |
| ATOM | 1803 | CG | ASP | 228 | 16.852 | 43.060 | 67.796 | | 30.68 | AAAA AAAA |
| ATOM | 1804 | | ASP | 228 | 17.182 | 42.576 | 66.690 | | 23.87 | AAAA |
| ATOM | 1805 | | ASP | 228 | 17.053 | 44.256 | 68.123 | | 25.02 | AAAA |
| ATOM | 1806 | С | ASP | 228 | 15.440 | 39.835 | 69.265 | 1.00 | 18.83 | AAAA |
| MOTA | 1807 | 0 | ASP | 228 | 16.298 | 39.002 | 69.536 | 1.00 | 16.28 | AAAA |
| MOTA | 1808 | N | ASN | 229. | 14.291 | 39.930 | 59.928 | | 20.73 | AAAA |
| MOTA | 1809 1810 | CA CB | ASN | 229 | 13.975 | 39.015 | 71.007 | | 21.75 | AAAA |
| ATOM ATOM | 1811 | CG | ASN ASN | 229 229 | 12.706 12.943 | 39.483 40.738 | 71.712 | | 19.46 27.14 | AAAA |
| ATOM | 1812 | | ASN | 229 | 13.588 | 40.738 | 73.556 | | 33.03 | AAAA AAAA |
| ATOM | 1813 | | ASN | 229 | 12.464 | 41.874 | 72.019 | | 21.35 | AAAA |
| MOTA | 1814 | С | ASN | 229 | 13.833 | 37.596 | 70.503 | | 18.47 | AAAA |
| ATOM | 1815 | 0 | ASN | 229 | 14.284 | 36.644 | | | 22.47 | AAAA |
| ATOM | 1816 | N | GLU | 230 | 13.252 | 37.454 | 69.319 | | 17.79 | AAAA |
| ATOM | 1817 1818 | CA CB | GLU | 230 · 230 | 13.081 | 36.125 | 68.748 | | 21.18 | AAAA |
| ATOM ATOM | 1819 | CG | GLU | 230 | 12.152 10.765 | 36.193 36.714 | 67.536 67.890 | | 20.54 28.98 | AAAA AAAA |
| ATOM | 1820 | CD | GLU | 230 | 9.870 | 36.816 | 66.677 | | 24.35 | AAAA |
| ATOM | 1821 | | GLU | 230 | 10.360 | 37.296 | 65.638 | | 22.00 | AAAA |
| MOTA | 1822 | | GLU | 230 | 8.683 | 36.443 | 66.772 | 1.00 | 24.99 | AAAA |
| ATOM | 1823 | C | GLU | 230 | 14.422 | 35.507 | 68.361 | | 16.89 | AAAA |
| ATOM | 1824 | 0 | GLU | 230 | 14.663 | 34.326 | 68.603 | | 19.45 | AAAA |
| MOTA | 1825 1826 | N CA | PHE | 231 231 | 15.305 | 36.305 | 67.772 | | 15.68 | AAAA |
| ATOM ATOM | 1827 | CB | PHE | 231 | 16.616 17.420 | 35.788 36.863 | 67.389 66.649 | | 15.78 13.22 | AAAA AAAA |
| ATOM | 1828 | CG | PHE | 231 | 18.719 | 36.361 | 66.069 | | 20.63 | AAAA |
| ATOM | 1829 | CD1 | | 231 | 18.723 | 35.445 | 65.016 | | 18.42 | AAAA |
| MOTA | 1830 | CD2 | PHE | 231 | 19.936 | 36.804 | 66.568 | | 21.10 | AAAA |
| MOTA | 1831 | CE1 | | 231 | 19.918 | 34.983 | 64.471 | 1.00 | 17.67 | AAAA |
| MOTA | 1832 | CE2 | | 231 | 21.144 | 36.346 | 66.029 | | 28.29 | AAAA |
| MOTA | 1833 | CZ | PHE | 231 | 21.130 | 35.431 | 64.976 | | 27.85 | AAAA |
| MOTA | 1834 | C | PHE | 231 | 17.385 | 35.332 | 68.636 | 1.00 | | AAAA |
| MOTA MOTA | 1835 1836 | O N | PHE | 231 232 | 17.869 17.495 | 34.201 36.204 | 68.702 69.636 | | 18.86 19.07 | AAAA AAAA |
| MOTA | 1837 | | LEU | 232 | 18.239 | 35.850 | 70.848 | | 17.39 | AAAA |
| ATOM | 1838 | | LEU | 232 | 18.415 | 37.078 | 71.737 | | 24.53 | AAAA |
| ATOM | 1839 | | LEU | 232 | 19.214 | 38.202 | 71.061 | 1.00 | 16.64 | AAAA |
| MOTA | 1840 | CD1 | | 232 | 19.134 | 39.449 | 71.934 | | 26.70 | AAAA |
| MOTA | 1841 | CD2 | | 232 | 20.659 | 37.806 | 70.810 | | 18.77 | AAAA |
| ATOM | 1842 | | LEU | 232 | 17.607 | 34.707 | 71.628 | 1.00 | | AAAA |
| ATOM | 1843 | | LEU | 232 | 18.309 | 33.904 | 72.217 | | 21.80 | AAAA |
| MOTA MOTA | 1844 1845 | | PHE PHE | 233 233 | 16.281 15.587 | 34.640 33.537 | 71.648 72.309 | 1.00 | | AAAA AAAA |
| ATOM | 1846 | | PHE | 233 | 14.074 | 33.663 | 72.309 | 1.00 | | AAAA |
| ATOM | 1847 | | PHE | 233 | 13.289 | 32.447 | 72.523 | | 21.40 | AAAA |
| ATOM | 1848 | CD1 | | 233 | 12.863 | 32.302 | 73.841 | 1.00 | | AAAA |
| | | | | ٠ | | | _ | | | |

| | | | | | 12 042 | 31.473 | 71.596 | 1.00 19.92 | AAAA |
|------|------|-----|--------|-----|----------|--------|---------|--------------|--------|
| ATOM | 1849 | CD2 | | 233 | | | 74.229 | 1.00 29.35 | AAAA |
| ATOM | 1850 | CE1 | PHE | 233 | 10.000 | | | 1.00 25.37 | AAAA |
| ATOM | 1851 | CE2 | PHE | 233 | 20 | | 73.283 | 1.00 30.28 | AAAA |
| ATOM | 1852 | CZ | PHE | 233 | | | 71.660 | 1.00 23.12 | AAAA |
| | 1853 | С | PHE | 233 | 10.01- | | | 1.00 18.35 | AAAA |
| MOTA | 1854 | Ō | PHE | 233 | | | 72.332 | 1.00 17.26 | AAAA |
| ATOM | 1855 | N | ALA | 234 | | J | 70.332 | 1.00 17.20 | AAAA |
| MOTA | _ | CA | ALA | 234 | 16.332 | | 69.562 | 1.00 17.67 | |
| MOTA | 1856 | | ALA | 234 | 16.085 | | 68.046 | 1.00 19.08 | AAAA |
| MOTA | 1857 | CB | | 234 | 17.786 | 30.641 | 69.800 | 1.00 16.31 | AAAA |
| MOTA | 1858 | C | ALA | 234 | 18.127 | 29.461 | 69.926 | 1.00 16.75 | AAAA |
| MOTA | 1859 | 0 | ALA | | 18.646 | 31.643 | 69.846 | 1.00 16.73 | AAAA |
| MOTA | 1860 | N | LEU | 235 | 20.074 | 31.411 | 70.051 | 1.00 19.14 | AAAA . |
| MOTA | 1861 | CA | LEU | 235 | 20.823 | 32.742 | 69.956 | 1.00 21.72 | AAAA |
| MOTA | 1862 | CB | LEU | 235 | 22.226 | 32.790 | 69.345 | 1.00 36.73 | AAAA |
| MOTA | 1863 | CG | LEU | 235 | 23.026 | 33.844 | 70.105 | 1.00 20.69 | AAAA |
| MOTA | 1864 | | LEU | 235 | | 31.426 | 69.393 | 1.00 22.96 | AAAA |
| MOTA | 1865 | CD2 | LEU | 235 | 22.917 | 30.776 | 71.421 | 1.00 18.71 | AAAA |
| ATOM | 1866 | С | LEU | 235 | 20.354 | 29.747 | 71.522 | 1.00 18.59 | AAAA |
| ATOM | 1867 | 0 | LEU | 235 | 21.028 | 29.747 | 72.479 | 1.00 25.43 | AAAA |
| MOTA | 1868 | N | GLU | 236 | 19.831 | 31.390 | 73.839 | 1.00 19.75 | AAAA |
| | 1869 | ÇA | GLU | 236 | 20.046 | 30.883 | | 1.00 23.18 | AAAA |
| ATOM | 1870 | CB | GLU | 236 | 19.335 | 31.777 | 74.860 | 1.00 38.53 | AAAA |
| ATOM | 1871 | CG | GLU | 236 | 19.725 | 33.229 | 74.777 | 1.00 42.42 | AAAA |
| ATOM | 1872 | CD | GLU | 236 | 18:857 | 34.119 | 75.648 | 1.00 42.42 | AAAA |
| MOTA | | OFI | GLU | 236 | 17.617 | 34.171 | 75.428 | 1.00 45.43 | AAAA |
| MOTA | 1873 | | GLU | 236 | 19.425 | 34.768 | 76.548 | 1.00 48.76 | AAAA |
| MOTA | 1874 | | GLU | 236 | 19.541 | 29.452 | 74.011 | 1.00 25.85 | AAAA |
| MOTA | 1875 | c | GLU | 236 | 20.222 | 28.603 | 74.597 | 1.00 21.36 | |
| MOTA | 1876 | 0 | | 237 | 18.343 | 29.193 | 73.501 | 1.00 23.16 | AAAA |
| MOTA | 1877 | Ň | LYS | 237 | 17.752 | 27.871 | 73.610 | 1.00 17.06 | AAAA |
| ATOM | 1878 | CA | LYS | 237 | 16.282 | 27.943 | 73.193 | 1.00 26.98 | AAAA |
| ATOM | 1879 | CB | LYS | | 15.483 | 26.711 | 73.519 | 1.00 52.00 | AAAA |
| MOTA | 1880 | CG | LYS | 237 | 14.078 | 27.110 | 73.932 | 1.00 56.40 | AAAA |
| MOTA | 1881 | CD | LYS | 237 | 14.131 | 27.979 | 75.183 | 1.00 52.03 | AAAA |
| ATOM | 1882 | CE | LYS | 237 | 12.782 | 28.421 | 75.614 | 1.00 55.53 | AAAA |
| ATOM | 1883 | NZ | LYS | 237 | | 26.827 | 72.785 | 1.00 18.46 | AAAA |
| ATOM | 1884 | С | LYS | 237 | 18.502 | 25.692 | 73.231 | 1.00 21.20 | AAAA |
| ATOM | 1885 | 0 | LYS | 237 | 18.691 | 27.187 | 71.578 | 1.00 21.28 | AAAA |
| MOTA | 1886 | N | SER | 238 | 18.932 | 26.208 | 70.776 | 1.00 16.47 | AAAA |
| ATOM | 1887 | CA | SER | 238 | 19.649 | | 69.307 | 1.00 19.75 | AAAA |
| ATOM | 1888 | CB | SER | 238 | 19.745 | 26.666 | 69.160 | | AAAA |
| ATOM | 1889 | OG | SER | 238 | 20.475 | 27.858 | 71.361 | | AAAA |
| | 1890 | C | SER | 238 | 21.039 | 25.923 | | | AAAA |
| MOTA | 1891 | ō | SER | 238 | 21.521 | 24.788 | 71.312 | | AAAA |
| MOTA | 1892 | N | LEU | 239 | 21.690 | 26.937 | 71.925 | | AAAA |
| MOTA | 1893 | CA | | 239 | 23.004 | 26.701 | | | AAAA |
| MOTA | | CB. | | 239 | 23.652 | 28.008 | 72.986 | | AAAA |
| MOTA | 1894 | CG | | 239 | 23.985 | 29.072 | 71.933 | | AAAA |
| MOTA | 1895 | | 1 LEU | 239 | 24.538 | 30.311 | 72.636 | 1.00 27.02 | AAAA |
| MOTA | 1896 | כט | 1 1150 | 239 | 25.010 | 28.556 | 70.933 | 1.00 20.31 | |
| ATOM | 1897 | | 2 LEU | 239 | 22.882 | 25.735 | 73.680 | 1.00 25.16 | AAAA |
| MOTA | 1898 | C | LEU | | 23.780 | 24.929 | 73.920 | 1.00 20.70 | AAAA |
| ATOM | 1899 | 0 | LEU | 239 | 21.768 | 25.800 | 74.398 | 1.00 24.93 | AAAA |
| MOTA | 1900 | | GLU | 240 | 21.570 | | | 1.00 25.72 | AAAA |
| MOTA | 1901 | CA | | 240 | 20.331 | | | 1 1.00 29.10 | AAAA |
| ATOM | 1902 | CB | | 240 | 20.011 | 24.531 | | 1.00 49.56 | AAAA |
| ATOM | 1903 | CG | GLU | 240 | 20.042 | | | | AAAA |
| ATOM | 1904 | CD | GLU | 240 | 19.053 | | | | AAAA |
| ATOM | | | 1 GLU | 240 | 17.935 | | | | AAAA |
| | | | | 240 | 19.400 | | | | AAAA |
| ATOM | 4447 | | GLU | 240 | 21.440 | | | | AAAA |
| MOTA | 4000 | _ | GLU | 240 | 21.951 | | | | AAAA |
| MOTA | | | ILE | 241 | 20.771 | 23.294 | | | AAAA |
| MOTA | | | | 241 | 20.598 | 21.97 | | 1 1.00 24.06 | AAAA |
| ATOM | | | | 241 | 19.705 | 22.039 | | | AAAA |
| atom | 1911 | | 2 ILE | 241 | 19.718 | 20.67 | B 71.32 | | AAAA |
| ATOM | 1912 | | 14 ILE | 241 | 18.28 | 22.43 | 3 72.43 | 9 1.00 28.60 | |
| ATOM | 1913 | | 1 ILE | 241 | 17.336 | | 0 71.25 | 7 1.00 27.04 | AAAA |
| ATOM | | CI | 1 ILE | 241 | . 1,.550 | | • | • | • |
| | | | • | | | | | | |
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| | | | | | - | | | | |
|------|--------|------|------------|------------|----------|------------------|------------------|--------------------------|--------------|
| ATOM | 191 | | ILE | 241 | 21.95 | 7 21.404 | 72.941 | 1.00 25.48 | AAAA |
| ATOM | | | IL | 241 | 22.24 | | | | AAAA |
| ATOM | | | VAI | 242 | 22.799 | | | 1.00 20.41 | |
| ATOM | 191 | 8 C. | A VAL | 242 | 24.116 | | | | AAAA |
| ATOM | 191 | 9 CE | 3 VAL | 242 | 24.853 | | | | AAAA AAAA |
| MOTA | 1920 | 0 0 | 31 VAL | 242 | 26.273 | | | | |
| ATOM | 192 | 1 CC | 2 VAL | 242 | 24.093 | | | | AAAA |
| ATOM | 1922 | 2 C | VAL | | 24.962 | | | 1.00 24.81 | AAAA |
| ATOM | 1923 | 3 0 | VAL | | 25.566 | | 73.235 | | AAAA |
| ATOM | 1924 | 1 N | LYS | | 24.989 | | | | AAAA |
| ATOM | 1925 | | | | 25.775 | | | | AAAA |
| ATOM | 1926 | | | | 25.599 | | | | AAAA |
| ATOM | 1927 | CG | | | 26.386 | | | | AAAA |
| ATOM | 1928 | | | _ | 26.022 | | | | AAAA |
| ATOM | 1929 | | | 243 | 26.407 | | | | AAAA |
| ATOM | 1930 | | | 243 | 26.045 | | | | AAAA |
| ATOM | 1931 | | LYS | 243 | 25.433 | | | | AAAA |
| ATOM | 1932 | | LYS | 243 | 26.321 | | 76.040 | | AAAA |
| ATOM | 1933 | | GLU | 244 | 24.161 | | | 1.00 35.44 | AAAA |
| ATOM | 1934 | | | 244 | 23.798 | | | | AAAA |
| ATOM | 1935 | | GLU | 244 | 22.288 | | | 1.00 37.54 | AAAA |
| ATOM | 1936 | | GLU | 244 | 21.735 | 19.260 20.459 | 77.048 | 1.00 35.34 | AAAA |
| ATOM | 1937 | | | 244 | 20.281 | | 77.816 | 1.00 55.88 | |
| ATOM | 1938 | | 1 GLU | 244 | 19.673 | 20.275 | 78.230 | 1.00 57.89 | AAAA |
| ATOM | 1939 | | 2 GLU | 244 | 19.753 | 21.246 | 78.738 | 1.00 60.60 | AAAA |
| ATOM | 1940 | c c | GLU | 244 | 24.231 | 19.152 | 78.062 | 1.00 57.73 | AAAA |
| ATOM | 1941 | ō | GLU | 244 | 24.294 | 18.034 | 76.102 | 1.00 38.17 | AAAA |
| ATOM | 1942 | N | VAL | 245 | . 24.541 | 16.978 | 76.727 | 1.00 38.46 | AAAA |
| MOTA | 1943 | CA | VAL | 245 | 24.933 | 18.124 | 74.817 | 1.00 30.29 | АААА |
| ATOM | 1944 | СВ | VAL | 245 | 23.984 | 16.958 16.778 | 74.042 | 1.00 29.17 | AAAA |
| MOTA | 1945 | | L VAL | 245 | 24.462 | 15.641 | 72.833 | 1.00 46.68 | AAAA |
| MOTA | 1946 | | VAL. | 245 | 22.581 | 16.488 | 71.942 | 1.00 53.09 | AAAA |
| ATOM | 1947 | c | VAL | 245 | 26.364 | 16.982 | 73.327 | 1.00 54.19 | AAAA |
| ATOM | 1948 | ō | VAL | 245 | 26.915 | 15.939 | 73.508 | 1.00 34.90 | AAAA |
| ATOM | 1949 | N | PHE | 246 | 26.980 | 18.156 | 73.164 | 1.00 34.73 | AAAA |
| ATOM | 1950 | CA | PHE | 246 | 28.324 | 18.256 | 73.465 | 1.00 29.22 | AAAA |
| ATOM | 1951 | CB | PHE | 246 | 28.178 | 18.800 | 72.897 71.464 | 1.00 29.17 | AAAA |
| ATOM | 1952 | CG | PHE | 246 | 29.384 | 18.588 | 70.585 | 1.00 30.42 | AAAA |
| ATOM | 1953 | | PHE | 246 | 29.695 | 17.326 | 70.097 | 1.00 25.62 1.00 28.89 | AAAA |
| ATOM | . 1954 | | PHE | 246 | 30.167 | 19.668 | 70.196 | 1.00 25.17 | AAAA |
| MOTA | 1955 | | PHE | 246 | 30.771 | 17.138 | 69.222 | 1.00 23.17 | AAAA |
| ATOM | 1956 | | PHE | 246 | 31.248 | 19.495 | 69.322 | 1.00 23.43 | AAAA |
| MOTA | 1957 | CZ | PHE | 246 | 31.549 | 18.236 | 68.835 | 1.00 22.40 | AAAA |
| MOTA | 1958 | C | PHE | 246 | 29.233 | 19.176 | 73.712 | 1.00 19.88 | AAAA |
| MOTA | 1959 | Ō | PHE | 246 | 28.867 | 20.312 | 74.002 | 1.00 23.38 | AAAA |
| ATOM | 1960 | N | GLU | 247 | 30.410 | 18.682 | 74.094 | 1.00 29.13 | AAAA |
| ATOM | 1961 | CA | GLU | 247 | 31.395 | 19.481 | 74.841 | 1.00 29.73 | AAAA |
| ATOM | 1962 | CB | GLU | 247 | 31.912 | 18.726 | 76.074 | 1.00 25.10 | AAAA |
| ATOM | 1963 | CG | GLU | 247 | 30.972 | 18.707 | 77.286 | 1.00 60.78 | AAAA |
| ATOM | 1964 | CD | GLU | 247 | 29.700 | 17.892 | 77.200 | 1.00 70.07 | AAAA |
| MOTA | 1965 | OE1 | | 247 | 28.913 | 18.220 | 76.165 | 1.00 70.07 | AAAA |
| ATOM | 1966 | | GLU | 247 | 29.481 | 16.920 | 77.835 | 1.00 76.80 | AAAA |
| MOTA | 1967 | С | GLU | 247 | 32.554 | 19.741 | 73.876 | 1.00 78.80 | AAAA |
| ATOM | 1968 | 0 | GLU | 247 | 33.490 | 18.946 | 73.778 | 1.00 28.90 | AAAA |
| MOTA | 1969 | N | PRO | 248 | 32.531 | 20.891 | 73.778 | 1.00 25.02 | AAAA |
| ATOM | 1970 | CD | PRO | 248 | 31.574 | 22.003 | 73.310 | 1.00 27.23 | AAAA |
| ATOM | 1971 | CA | PRO | 248 | 33.566 | 21.249 | 72.209 | | AAAA |
| MOTA | 1972 | СВ | PRO | 248 | 33.050 | 22.575 | | 1.00 28.06 | AAAA |
| ATOM | 1973 | | PRO | 248 | 31.551 | 22.512 | 71.639 | 1.00 28.11 | AAAA |
| ATOM | 1974 | _ | PRO | 248 | 34.968 | | 71.897 | 1.00 34.57 | AAAA |
| ATOM | 1975 | | PRO | 248 | 35.132 | 21.416 21.897 | 72.770 | 1.00 23.87 | AAAA |
| ATOM | 1976 | | GLU | 249 | 35.965 | | 73.887 | 1.00 24.05 | AAAA |
| ATOM | 1977 | | GLU | 249 | | 21.013 | 71.983 | 1.00 24.34 | AAAA |
| | | | | | 37.366 | 21.195 | 72.355 | 1.00 25.98 | AAAA |
| ATOM | | | GLU | 249 249 | 38.275 | 20.166 | 71.679 | 1.00 22.07 | AAAA |
| ATOM | | | GLU GLU | 249 | 38.046 | 18.726 | 72.116 | 1.00 33.40 | AAAA |
| ATOM | +500 | CD . | GLU | 243 | 39.005 | 17.767 | 71.445 | 1.00 29.15 | AAAA |
| | | - | | | | | | | _ |

| | | 077 | OT 11 | 249 | 39.071 | 17.770 | 70.199 | 1.00 27.62 | AAAA |
|--------|------|-----|-------|-------------|----------------|---------------------|--------|------------|------|
| ATOM | 1981 | OE1 | | | 39.694 | 17.004 | 72.161 | 1.00 26.19 | AAAA |
| MOTA | 1982 | OE2 | | 249 | | | 71.786 | 1.00 26.04 | AAAA |
| MOTA | 1983 | С | GLU | 249 | 37.692 | 22.561 | | | AAAA |
| MOTA | 1984 | 0 | GLU | 249 | 38.582 | 23.271 | 72.262 | 1.00 26.39 | |
| | 1985 | Ŋ | VAL | 250 | 36.953 | 22.921 | 70.744 | 1.00 23.83 | AAAA |
| ATOM | | CA | VAL | 250 | 37.151 | 24.197 | 70.086 | 1.00 19.67 | AAAA |
| MOTA | 1986 | | | | 38.438 | 24.178 | 69.210 | 1.00 20.88 | AAAA |
| ATOM | 1987 | | _VAL | 250 | + · · · | 23.117 | 68.128 | 1.00 18.18 | AAAA |
| MOTA | 1988 | CG1 | | 250 | 38.348 | | | 1.00 16.71 | AAAA |
| ATOM | 1989 | CG2 | VAL | .250 | 38.647 | 25.530 | 68.591 | | |
| ATOM | 1990 | С | VAL | 250 | 35.946 | 24.483 | 69.207 | 1.00 20.78 | AAAA |
| | | ō | VAL | 250 | . 35.299 | 23.556 | 68.746 | 1.00 19.60 | AAAA |
| ATOM . | 1991 | | | 251 | 35.633 | 25.757 | 69.000 | 1.00 18.75 | AAAA |
| MOTA | 1992 | N | TYR | | 34.497 | 26.109 | 68.153 | 1.00 22.44 | AAAA |
| MOTA | 1993 | CA | TYR | 251 | | | 69.022 | 1.00 16.57 | AAAA |
| ATOM | 1994 | CB | TYR | 251 | 33.261 | 26.437 | | 1.00 22.36 | AAAA |
| ATOM | 1995 | CG | TYR | -251 | 33.207 | 27.856 | 69.575 | | |
| | 1996 | | TYR . | 251 | 32.654 | 28.896 | 68.823 | 1.00 18.12 | AAAA |
| MOTA | | | TYR | 251 | 32.612 | 30.185 | 69.308 | 1.00 20.40 | AAAA |
| MOTA | 1997 | | | | 33.715 | 28.160 | 70.842 | 1.00 20.04 | AAAA |
| MOTA | 1998 | | TYR | 251 | 33.676 | 29.475 | 71.349 | 1.00 16.60 | AAAA |
| ATOM | 1999 | CE2 | TYR | 251 | | | 70.573 | 1.00 14.68 | AAAA |
| MOTA | 2000 | CZ | TYR | 251 | 33.128 | 30.473 | | | AAAA |
| ATOM | 2001 | OH | TYR | 251 | 33.100 | 31.780 | 71.011 | 1.00 21.79 | |
| | 2002 | С | TYR | 251 | 34.811 | 27.294 | 67.236 | 1.00 20.28 | AAAA |
| MOTA | | | TYR | 251 | 35.695 | 28.107 | 67.525 | 1.00 19.91 | AAAA |
| MOTA | 2003 | 0 | | | 34.097 | 27.360 | 66.109 | 1.00 17.90 | AAAA |
| ATOM | 2004 | N | LEU | 252 | | 28.466 | 65.161 | 1.00 18.58 | AAAA |
| ATOM | 2005 | CA | LEU | 252 | 34.216 | | | 1.00 17.55 | AAAA |
| ATOM | 2006 | CB | LEU | 252 | 34.679 | 28.001 | 63.767 | 1.00 17.33 | AAAA |
| ATOM | 2007 | CG | LEU | 252 | 36.028 | 27.290 | 63.718 | 1.00 23.36 | |
| | 2008 | | LEU | 252 | 35.819 | 25.820 | 64.017 | 1.00 27.78 | AAAA |
| ATOM | | | LEU | 252 | 36.631 | 27.440 | 62.331 | 1.00 27.29 | AAAA |
| MOTA | 2009 | | | | 32.816 | 29.049 | 65.052 | 1.00 15.49 | AAAA |
| ATOM | 2010 | С | LEU | 252 | | 28.320 | 65.120 | 1.00 18.82 | AAAA |
| MOTA | 2011 | 0 | LEU | | 31.819 | | 64.891 | 1.00 16.80 | AAAA |
| ATOM | 2012 | N | LEU | 253 | 32.756 | 30.360 | | 1.00 17.50 | AAAA |
| ATOM | 2013 | CA | LEU | 253 | 31.498 | 31.105 | 64.817 | | AAAA |
| | 2014 | CB | LEU | 253 | 31.379 | 31. 9 87 | 66.073 | 1.00 15.49 | |
| ATOM | | ĊG | LEU | 253 | 30.326 | 33.085 | 66.165 | 1.00 17.75 | AAAA |
| MOTA | 2015 | | | 253 | 28.946 | 32.438 | 66.172 | 1.00 20.85 | AAAA |
| MOTA | 2016 | | LEU | | 30.536 | 33.897 | 67.464 | 1.00 19.05 | AAAA |
| MOTA | 2017 | | LEU | 253 | | 31.985 | 63.580 | 1.00 20.22 | AAAA |
| ATOM | 2018 | С | LEU | 253 | 31.516 | | 63.371 | 1.00 18.14 | AAAA |
| ATOM | 2019 | 0 | LEU | 253 | 32.474 | 32.727 | - | 1.00 16.50 | AAAA |
| MOTA | 2020 | N | GLN | 254 | 30.466 | 31.913 | 62.765 | | AAAA |
| | 2021 | CA | GLN | 254 | 30.411 | 32.730 | 61.556 | 1.00 16.48 | |
| ATOM | | CB | GLN | 254 | 30.085 | 31.863 | 60.312 | 1.00 25.58 | AAAA |
| ATOM | 2022 | | | 254 | 28.647 | 31.798 | 59.871 | 1.00 36.40 | AAAA |
| MOTA | 2023 | CG | GLN | | 28.337 | 32.728 | | 1.00 33.18 | AAAA |
| ATOM | 2024 | CD | GLN | 254 | | | 57.546 | 1.00 21.05 | AAAA |
| MOTA | 2025 | OE1 | GLN | 254 | 28.744 | 32.487 | | 1.00 22.85 | AAAA |
| ATOM | 2026 | NE2 | GLN | 254 | 27.613 | 33.799 | | 1.00 22.03 | AAAA |
| | 2027 | С | GLN | 254 | 29.384 | 33.816 | | 1.00 16.12 | AAAA |
| ATOM | 2028 | | GLN | 254 | 28.282 | 33.577 | 62.364 | 1.00 13.97 | |
| MOTA | | | | 255 | 29.768 | 35.032 | 61.468 | 1.00 14.42 | AAAA |
| ATOM | 2029 | N | LEU | | 28.988 | 36.215 | | 1.00 17.99 | AAAA |
| ATOM | 2030 | CA | LEU | 255 | | | | 1.00 20.68 | AAAA |
| ATOM | 2031 | CB | LEU | 255 | 29.834 | 37.070 | | 1.00 22.90 | AAAA |
| ATOM | 2032 | CG | LEU | 255 | 30.240 | 36.283 | | | AAAA |
| | 2033 | | LEU | 255 | 31.446 | 36.906 | | 1.00 29.36 | |
| MOTA | | | LEU | 255 | 29.042 | 36.214 | 64.900 | 1.00 14.80 | AAAA |
| ATOM | 2034 | | | | 28.541 | | 60.594 | 1.00 19.32 | AAAA |
| ATOM | 2035 | c | LEU | 255 | 28.838 | 38.260 | | 1.00 21.23 | AAAA |
| ATOM | 2036 | 0 | LEU | 255 | | | | 1.00 17.21 | AAAA |
| MOTA | 2037 | N | GLY | 256 | 27.827 | | | | AAAA |
| ATOM | 2038 | CA | GLY | 256 | 27.347 | | | 1.00 13.04 | AAAA |
| | 2039 | C | GLY | 256 | 26.413 | 38.348 | 59.028 | | |
| MOTA | | | GLY | 256 | 25.717 | | | | AAAA |
| Mota | 2040 | 0 | | | 26.389 | | | 1.00 19.72 | AAAA |
| ATOM | 2041 | N | THR | 257 | | | | | AAAA |
| ATOM | 2042 | CA | THR | 257 | 25.536 | | | 1.00 14.02 | AAAA |
| ATOM | 2043 | CB | THR | 25 7 | 26.242 | | | | AAAA |
| | 2044 | | THR | 257 | 26.538 | 42.187 | | T.00 11.30 | AAAA |
| MOTA | | | THR | 257 | 27.543 | 42.009 | 59.392 | 1.00 19.67 | |
| ATOM | 2045 | CG2 | | | 24.199 | | 58.053 | 1.00 20.58 | AAAA |
| 3 moM | 2046 | (- | THE | 231 | 44.47 | | | | |

| MOTA | _ | | THE | | 23.40 | 3 41.545 | 58.266 | 1.00 14.59 | 7272 |
|------|------|-------|-------|-------|--------|----------|--------|--------------|--------|
| MOTA | | 8 N | ASE | 258 | 23.92 | 7 39.639 | | | AAAA |
| MOTA | | 9 CA | ASF | 258 | 22.65 | | | | AAAA |
| ATOM | 205 | 0 CB | ASP | 258 | 22.60 | | 55.388 | | AAAA |
| MOTA | 205 | 1 CG | | | 23.03 | | | | AAAA |
| ATOM | | | 1 ASP | | 23.22 | | | | AAAA |
| ATOM | | | 2 ASP | | | | - | | AAAA |
| MOTA | | | | | 23.187 | | | 1.00 18.12 | AAAA |
| | | | ASP | | 21.396 | | | | AAAA |
| AŢOM | | | ASP | | 20.300 | 39.781 | 56.897 | 1.00 22.52 | AAAA |
| ATOM | 205 | 6 N | PRO | 259 | 21.510 | | | | |
| ATOM | 205 | 7 CD | PRO | 259 | 22.614 | | | | AAAA |
| ATOM | 205 | B CA | PRO | 259 | 20.281 | | 59.482 | 1.00 21.24 | AAAA |
| ATOM | 205 | 9 CB | PRO | 259 | 20.710 | | 50.40Z | 1.00 21.24 | AAAA |
| ATOM | 206 | | PRO | 259 | 22.174 | | | - 1.00 21.18 | AAAA |
| ATOM | 206 | | PRO | 259 | | | | 1.00 36.11 | AAAA |
| ATOM | 2062 | | | | 19.705 | | | | AAAA |
| | | | PRO | 259 | 18.572 | | | 1.00 19.25 | -AAAA |
| ATOM | 2063 | _ | LEU | 260 | 20.473 | 41.591 | 59.571 | 1.00 18.75 | AAAA |
| ATOM | 2064 | | LEU | 260 | 20.023 | 42.949 | 59.875 | 1.00 22.16 | AAAA |
| ATOM | 2065 | | LEU | 260 | 21.202 | 43.935 | | 1.00 20.35 | AAAA |
| MOTA | 2066 | CG | LEU. | . 260 | 22.403 | | | 1.00 21.82 | |
| MOTA | 2067 | CD1 | LEU | 260 | 23.604 | | 60.253 | 1.00 21.82 | AAAA |
| ATOM | 2068 | CD2 | LEU | 260 | 22.032 | | | | AAAA |
| MOTA | 2069 | | LEU | 260 | 18.876 | | 62.123 | 1.00 19.18 | AAAA |
| ATOM | 2070 | | LEU | 260 | | | 59.014 | 1.00 24.16 | AAAA |
| ATOM | 2071 | | LEU | | 18.742 | 43.144 | 57.826 | 1.00 21.69 | AAAA |
| ATOM | 2072 | | | 2.61 | 18.049 | 44.300 | 59.634 | 1.00 19.54 | AAAA |
| | 2072 | - | LEU | 261 | 16.903 | 44.913 | 58.965 | 1.00 17.34 | AAAA |
| ATOM | | | LEU | 261 | 16.285 | 45.967 | 59.892 | 1.00 19.96 | AAAA |
| ATOM | 2074 | | LEU | 261 | 15.204 | 46.879 | 59.300 | 1.00 29.99 | AAAA |
| ATOM | 2075 | | LEU | 261 | 14.080 | 46.040 | 58.732 | 1.00 33.66 | AAAA |
| MOTA | 2076 | CD2 | LEU | 261 | 14.682 | 47.819 | 60.376 | 1.00 44.71 | AAAA |
| MOTA | 2077 | С | LEU | 261 | 17.262 | 45.550 | 57.620 | 1.00 18.11 | AAAA |
| MOTA | 2078 | 0 | LEU | 261 | 16.539 | 45.386 | 56.634 | 1.00 19.02 | |
| ATOM | 2079 | N | GLU | 262 | 18.391 | 46.249 | 57.566 | 1.00 19.02 | AAAA |
| ATOM | 2080 | CA | GLU | 262 - | 18.802 | 46.921 | | | AAAA |
| ATOM | 2081 | CB | GLU | 262 | 19.875 | | 56.338 | 1.00 18.46 | AAAA |
| ATOM | 2082 | CG | GLU | 262 | | 47.965 | 56.641 | 1.00 22.01 | AAAA |
| ATOM | 2083 | CD | GLU | | 19.365 | 49.136 | 57.443 | 1.00 22.94 | AAAA |
| ATOM | 2084 | | GLU | 262 | 19.434 | 48.902 | 58.927 | 1.00 23.11 | AAAA |
| ATOM | | | | 262 | 19.668 | 47.748 | 59.357 | 1.00 24.58 | AAAA |
| | 2085 | | GLU | 262 | 19.238 | 49.883 | 59.667 | 1.00 27.06 | AAAA |
| ATOM | 2086 | C | GLU | 262 | 19.281 | 46.034 | 55.197 | 1.00 25.65 | AAAA |
| ATOM | 2087 | 0 | GLU | 262 | 19.446 | 46.510 | 54.070 | 1.00 25.49 | AAAA |
| ATOM | 2088 | N | ASP | 263 | 19.501 | 44.750 | 55.467 | 1.00 22.45 | AAAA |
| ATOM | 2089 | CA | ASP | 263 | 19.959 | 43.851 | 54.418 | 1.00 15.93 | AAAA |
| ATOM | 2090 | CB | ASP | 263 | 20.981 | 42.859 | 54.988 | 1.00 18.99 | AAAA |
| ATOM | 2091 | CG | ASP | 263 | 21.706 | 42.081 | 53.907 | 1.00 22.21 | |
| ATOM | 2092 | OD1 | ASP | 263 | 22.876 | 41.730 | 54.139 | 1.00 23.19 | AAAA |
| ATOM | 2093 | OD2 | ASP | 263 | 21.112 | 41.809 | 52.838 | | AAAA |
| ATOM | 2094 | | ASP | 263 | 18.733 | 43.165 | | 1.00 25.02 | AAAA . |
| ATOM | 2095 | | ASP | 263 | 18.012 | | 53.837 | 1.00 22.32 | AAAA |
| ATOM | 2096 | | TYR | 264 | | 42.419 | 54.519 | 1.00 18.50 | AAAA |
| ATOM | 2097 | | | | 18.500 | 43.447 | 52.564 | 1.00 25.21 | AAAA |
| | | - | TYR | 264 | 17.339 | 42.936 | 51.865 | 1.00 29.92 | AAAA |
| ATOM | 2098 | | TYR | 264 | 17.077 | 43.776 | 50.596 | 1.00 38.48 | AAAA |
| MOTA | 2099 | | TYR | 264 | 17.910 | 43.431 | 49.379 | 1.00 54.09 | AAAA |
| MOTA | 2100 | CD1 | | 264 | 17.677 | 42.249 | 48.660 | 1.00 69.38 | AAAA |
| MOTA | 2101 | CE1 | | 264 | 18.420 | 41.930 | 47.526 | 1.00 68.71 | AAAA |
| ATOM | 2102 | CD2 | TYR . | 264 | 18.915 | 44.286 | 48.928 | 1.00 66.09 | AAAA |
| MOTA | 2103 | CE2 | ryr | 264 | 19.670 | 43.975 | 47.788 | 1.00 74.50 | |
| ATOM | 2104 | | . YR | 264 | 19.415 | 42.794 | 47.094 | 1.00 74.50 | AAAA |
| MOTA | 2105 | | ryr | 264 | 20.154 | 42.472 | | | AAAA |
| MOTA | 2106 | | TYR | 264 | 17.445 | | 45.975 | 1.00 71.96 | AAAA |
| ATOM | 2107 | | TYR | 264 | | 41.461 | 51.532 | 1.00 29.55 | AAAA |
| ATOM | 2107 | | | | 16.448 | 40.839 | 51.190 | 1.00 30.11 | AAAA |
| | | | .EU | 265 | 18.639 | 40.891 | 51.629 | 1.00 24.45 | AAAA |
| ATOM | | | .EU | 265 | 18.753 | 39.476 | 51.337 | 1.00 25.36 | AAAA |
| ATOM | | | .EU | 265 | 20.186 | 39.089 | 50.969 | 1.00 29.81 | AAAA |
| ATOM | | | .EU | 265 | 20.509 | 39.510 | 49.531 | 1.00 34.43 | AAAA |
| ATOM | 2112 | CD1 L | EU | 265 | 21.847 | 38.930 | 49.100 | 1.00 44.38 | AAAA |
| | | • • | | • • • | | | • | | |

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| | | | | · | 10 400 | 38,990 | 48,603 | 1.00 46.72 | AAAA |
|-------|------|------|------------|-------|--------|---------|--------|-------------|------|
| MOTA | 2113 | CD2 | | 265 | 19.422 | 38.585 | | 1.00 22.33 | AAAA |
| MOTA | 2114 | С | LEU | 265 | 18.209 | 37.364 | | 1.00 23.48 | AAAA |
| MOTA | 2115 | 0 | LEU | 265 | 18.279 | | | 1.00 17.50 | AAAA |
| ATOM | 2116 | N | SER | 266 | 17.677 | 39.194 | | 1.00 19.69 | AAAA |
| MOTA | 2117 | CA | SER | 266 | 17.055 | 38.398 | 55.845 | 1.00 20.73 | AAAA |
| MOTA | 2118 | CB | SER | 266 | 17.912 | 38.314 | | 1.00 22.81 | AAAA |
| ATOM | 2119 | OG | SER | 266 | 17.696 | 39.442 | 56.684 | 1.00 19.75 | AAAA |
| MOTA | 2120 | С | SER | 266 | 15.739 | 39.048 | 54.950 | 1.00 23.66 | AAAA |
| ATOM | 2121 | 0 | SER | 266 | 15.572 | 40.265 | 54.840 | 1.00 23.00 | AAAA |
| ATOM | 2122 | N | LYS | 267 | 14.799 | 38.229 | 55.402 | 1.00 20.64 | AAAA |
| MOTA | 2123 | CA | LYS | 267 | 13.527 | 38.759 | 55.851 | 1.00 20.96 | AAAA |
| MOTA | 2124 | CB | LYS | 267 | 12.397 | 37.787 | 55.513 | 1.00 25.60 | AAAA |
| MOTA | 2125 | CG | LYS | 267 | 12.269 | 37.536 | 54.025 | 1.00 23.00 | AAAA |
| MOTA. | 2126 | CD | LYS | 267 | 12.095 | 38.823 | 53.259 | 1.00 38.49 | AAAA |
| ATOM | 2127 | CE | LYS | 267 | 11.985 | 38.540 | 51.772 | 1.00 33.11 | AAAA |
| ATOM | 2128 | NZ | LYS | 267 | 11.954 | 39.793 | 50.991 | 1.00 33.11 | AAAA |
| ATOM | 2129 | С | LYS | 267 | 13.601 | 38.987 | 57.365 | 1.00 25.38 | AAAA |
| ATOM | 2130 | 0 | LYS | 267 | 12.584 | 39.192 | 58.017 | | AAAA |
| MOTA | 2131 | N | PHE | 268 | 14.814 | 38.937 | 57.915 | 1.00 18.98 | AAAA |
| ATOM | 2132 | CA | PHE | 268 | 15.034 | 39.182 | 59.345 | 1.00 18.50 | AAAA |
| ATOM | 2133 | CB | PHE | 268 | 16.328 | 38.510 | 59.833 | 1.00 20.91 | |
| MOTA | 2134 | CG | PHE | 268 | 16.252 | 37.006 | 59.967 | 1.00 16.96 | AAAA |
| ATOM | 2135 | | PHE | 268 | 17.374 | 36.290 | 60.415 | 1.00 16.61 | AAAA |
| ATOM | 2136 | | PHE | 268 | 15.081 | 36.303 | 59.682 | 1.00 18.13 | AAAA |
| MOTA | 2137 | | PHE | 268 | 17.331 | 34.904 | 60.581 | 1.00 14.81 | AAAA |
| | 2138 | | PHE | 268 | 15.027 | 34.900 | 59.849 | 1.00 17.45 | AAAA |
| MOTA | 2139 | CZ | PHE | 268 | 16.144 | 34.208 | 60.296 | 1.00 16.01 | AAAA |
| MOTA | 2140 | c | PHE | 268 | 15.179 | 40.699 | 59.510 | 1.00 18.33 | AAAA |
| MOTA | 2141 | õ | PHE | 268 | 15.733 | 41.371 | 58.644 | 1.00 18.28 | AAAA |
| MOTA | 2142 | N | ASN | 269 | 14.679 | 41.236 | 60.613 | 1.00 21.04 | AAAA |
| ATOM | 2143 | CA | ASN | 269 | 14.763 | 42.675 | 60.859 | 1.00 22.89 | AAAA |
| MOTA | 2144 | CB | ASN | 269 | 13.365 | 43.298 | 60.940 | 1.00 20.55 | AAAA |
| MOTA | 2145 | CG | ASN | 269 | 12.551 | 43.071. | | 1.00 26.13 | AAAA |
| MOTA | 2145 | | ASN | 269 | 13.060 | 43:192 | 58.571 | 1.00 29.17 | AAAA |
| MOTA | 2147 | ND2 | | 269 | 11.268 | 42.767 | 59.860 | 1.00 28.26 | AAAA |
| MOTA | 2148 | C | ASN | 269 | 15,493 | 42.967 | 62.159 | 1.00 19.00 | AAAA |
| MOTA | 2149 | ò | ASN | 269 | 14.984 | 43.683 | 63.019 | 1.00 21.85 | AAAA |
| ATOM | 2150 | N | LEU | 270 | 16.695 | 42.435 | 62.298 | 1.00 17.71 | AAAA |
| MOTA | 2151 | CA | LEU | 270 | 17,441 | 42.642 | 63.521 | 1.00 18.57 | AAAA |
| MOTA | 2152 | CB | LEU | 270 | 18.441 | 41.507 | 63.712 | 1.00 18.95 | AAAA |
| MOTA | 2153 | CG | LEU | 270 | 17.945 | 40.058 | 63.631 | 1.00 20.54 | AAAA |
| MOTA | 2154 | | LEU | 270 | 19.070 | 39.174 | 64.152 | 1.00 14.19 | AAAA |
| MOTA | 2155 | | LEU | 270 | 16.679 | 39.853 | 64.465 | 1.00 19.05 | AAAA |
| ATOM | 2156 | C | LEU | 270 | 18.203 | 43.971 | 63.583 | 1.00 22.83 | AAAA |
| ATOM | 2157 | Ö | LEU | 270 | 18.409 | 44.643 | 62.560 | 1.00 18.25 | AAAA |
| MOTA | 2158 | N | SER | 271 | 18.621 | 44.318 | 64.799 | 1.00 20.95 | AAAA |
| MOTA | 2159 | CA | SER | 271 | 19.414 | 45.518 | | 1.00 18.28 | AAAA |
| MOTA | 2160 | CB | SER | 271 | 18.985 | 46.150 | | 1.00 18.73 | AAAA |
| MOTA | 2161 | OG | SER | 271 | 19.347 | 45.327 | 67.512 | 1.00 22.28 | AAAA |
| MOTA | 2162 | C | SER | 271 | 20.875 | 45.073 | | 1.00 19.98 | AAAA |
| ATOM | 2163 | ō | SER | 271 | 21.122 | 43.899 | 65.537 | 1.00 18.82 | AAAA |
| ATOM | 2164 | Ŋ | ASN | 272 | 21.828 | 45.994 | 65.020 | 1.00 16.17 | AAAA |
| MOTA | 2165 | CA | ASN | 272 | 23.270 | | 65.145 | 1.00 20.70 | AAAA |
| MOTA | | CB | ASN | 272 | 24.176 | | | 1.00 37.49 | AAAA |
| ATOM | 2166 | CG | ASN | 272 | 24,161 | | 63.483 | 1.00 54.53 | AAAA |
| ATOM | 2167 | | LASN | 272 | 24.702 | | 63.199 | 1.00 45.61 | AAAA |
| ATOM | 2168 | | 2 ASN | | 23.576 | | 62.579 | 1.00 60.55 | AAAA |
| MOTA | 2169 | C VD | ASN ASN | | 23.586 | | | 1.00 18.03 | AAAA |
| ATOM | 2170 | | ASN | | 24.545 | | | 1.00 18.58 | AAAA |
| MOTA | 2171 | O | VAL | | 22.831 | | | 1.00 19.57 | AAAA |
| MOTA | 2172 | N | VAL | | 23.053 | | | 1.00 22.12 | AAAA |
| ATOM | 2173 | CA | | | 22.345 | | | 1.00 26.91 | AAAA |
| MOTA | 2174 | CB | VAL | | 22.440 | | | .1.00 39.69 | AAAA |
| ATOM | 2175 | | 1 VAL | | 23.034 | | | 1.00 34.73 | AAAA |
| MOTA | 2176 | | 2 VAL | | 22.636 | _ | | 1.00 22.06 | AAAA |
| MOTA | 2177 | C | VAL | | 23.249 | | | 00 | AAAA |
| MOTA | 2178 | 0 | VAL | . 213 | | | • | • | • |
| | | | | | | | | | |

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| | | | _ | | | | | | |
|--------------|----------------|------|------------|--------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | | | | • | 21.60 | 1 43.747 | 7 68.713 | 1.00 21.79 | AAAA |
| ATOM | | | A AL | | 21.20 | 7 42.383 | 69.035 | 1.00 21.31 | AAAA |
| ATOM | | | B ALA | - | 19.80 | 6 42.092 | 8 68.475 | 1.00 18.95 | AAAA |
| ATOM | | | | | 22.259 | 9 41.451 | 68.400 | 1.00 17.83 | AAAA |
| ATOM | | | | _ | 22.569 | 9 40.389 | 68.947 | | AAAA |
| ATOM | | _ | | | 22.798 | 3 41.859 | | 1.00 16.01 | AAAA |
| ATOM | | - | | 275 | 23.828 | 3 41.089 | 66.536 | 1.00 16.46 | AAAA |
| MOTA | | | B PHE | 275 | 24.220 | 41.835 | | | AAAA |
| ATOM | 218 | 7 C | G PHE | 275 | 25.363 | | | | |
| MOTA | 218 | | D1 PHE | | 25.209 | | | | AAAA |
| ATOM | | 9 C | D2 PHE | 275 | 26.590 | | | 1.00 22.40 | AAAA |
| ATOM | · 219 | 0 C | E1 PHE | 275 | 26.266 | | | 1.00 28.74 | AAAA |
| MOTA | 219 | 1 C | E2 PHE | 275 | 27.654 | | | | AAAA |
| ATOM | 219 | 2 C | Z PHE | 275 | 27.489 | 40.181 | | 1.00 24.63 | AAAA AAAA |
| MOTA | | | PHE | 275 | | | | 1.00 25.06 | |
| MOTA | 219 | | PHE | 275 | 25.619 | | _ | 1.00 19.71 | AAAA AAAA |
| MOTA | 219 | | LEU | 2 7 6 | 25.366 | | | 1.00 17.49 | AAAA |
| ATOM | 219 | 6 C/ | A LEU | 276 | 26.482 | | | 1.00 24.23 | AAAA |
| ATOM | 219 | 7 CI | LEU | 276 | 26.736 | | | 1.00 20.44 | |
| ATOM | 219 | 8 C0 | LEU | 276 | 28.001 | | | 1.00 39.65 | AAAA AAAA |
| ATOM | 219 | 9 CI | 1 LEU | 276 | 27.948 | | | 1.00 29.65 | |
| ATOM | 2200 | O CI | 2 LEU | 276 | 28.102 | | 71.460 | 1.00 32.41 | AAAA AAAA |
| MOTA | 2203 | | LEU | 276 | 26.180 | | 70.262 | 1.00 18.88 | AAAA |
| MOTA | 2202 | | LEU | 276 | 27.045 | | 70.727 | 1.00 17.99 | AAAA |
| MOTA | 2203 | | LYS | 277 | 24.968 | 41.374 | 70.805 | 1.00 19.67 | AAAA |
| ATOM | 2204 | | | 277 | 24.644 | 40.552 | 71.964 | 1.00 21.33 | AAAA |
| ATOM | 2205 | _ | | 277 | 23.265 | 40.888 | 72.532 | 1.00 23.84 | AAAA |
| MOTA | 2206 | | - | 277 | 23.247 | 42.126 | 73.366 | 1.00 40.87 | AAAA |
| ATOM | 2207 | | | 277 | 22.069 | 42.086 | 74.325 | 1.00 54.73 | AAAA |
| MOTA | 2208 | | | 277 | 22.172 | 40.884 | 75.254 | 1.00 58.85 | AAAA |
| ATOM | 2209 | | LYS | 277 | 21.051 | 40.844 | 76.228 | 1.00 55,34 | AAAA |
| ATOM | 2210 | | LYS | 277 | 24.695 | 39.068 | 71.660 | 1.00 22.12 | AAAA |
| MOTA | 2211 | | LYS | 277 | 25.074 | 38.264 | 72.513 | 1.00 22.19 | AAAA |
| ATOM | 2212 | | ALA | 278 | 24.311 | 38.700 | 70.441 | 1.00 20.23 | AAAA |
| ATOM ATOM | . 2213 2214 | | λLA | 278 | 24.325 | 37.291 | 70.039 | 1.00 17.06 | AAAA |
| ATOM | 2215 | | ALA ALA | 278 | 23.798 | 37.154 | 68.589 | 1.00 19.27 | AAAA |
| MOTA | 2216 | | ALA | 278 278 | 25.760 | 36.767 | 70.127 | 1.00 16.94 | AAAA |
| ATOM | 2217 | | PHE | 278 279 | 26.035 | 35.676 | 70.648 | 1.00 14.93 | AAAA |
| ATOM | 2218 | CA | PHE | 279 279 | 26.679 | 37.564 | 69.606 | 1.00 18.88 | AAAA |
| ATOM | 2219 | СВ | PHE | 279 | 28.099 | 37.231 | 69.626 | 1.00 21.01 | AAAA |
| ATOM | 2220 | CG | PHE | 279 | 28.880 30.370 | 38.392 | 68.998 | 1.00 16.79 | AAAA |
| ATOM | 2221 | | PHE | 279 | 31.062 | 38.264 37.272 | 69.120 | 1.00 20.23 | AAAA |
| ATOM | 2222 | | PHE | 279 | 31.088 | 39.159 | 68.423 | 1.00 21.61 | AAAA |
| ATOM | 2223 | | PHE | 279 | 32.461 | 37.185 | 69.905 | 1.00 23.24 | AAAA |
| ATOM | 2224 | | PHE | 279 | 32.480 | 39.081 | 68.509 | 1.00 30.98 | AAAA |
| ATOM | 2225 | CZ | PHE | 279 | 33.169 | 38.095 | 69.995 69.295 | 1.00 24.82 | AAAA |
| ATOM | 2226 | С | PHE | 279 | 28.576 | 36.995 | 71:067 | 1.00 30.27 1.00 25.48 | AAAA |
| ATOM | 2227 | 0 | PHE | 279 | 29.275 | 36.016 | 71.362 | 1.00 25.48 | AAAA |
| MOTA | 2228 | N | ASN | 280 | 28.194 | 37.898 | 71.962 | 1.00 22.30 | AAAA |
| ATOM | 2229 | CA | ASN | 280 | 28.599 | 37.777 | 73.352 | 1.00 24.49 | AAAA AAAA |
| ATOM | 2230 | CB | ASN | 280 | 28.391 | 39.109 | 74.080 | 1.00 27.17 | AAAA |
| ATOM | 2231 | CG | ASN | 280 | 29.344 | 40.183 | 73.578 | 1.00 20.88 | AAAA |
| ATOM | 2232 | OD1 | ASN | 280 | 30.503 | 39.897 | 73.273 | 1.00 22.95 | AAAA |
| MOTA | 2233 | ND2 | ASN | 280 | 28.875 | 41.421 | 73.522 | 1.00 27.85 | AAAA |
| MOTA | 2234 | С | ASN | 280 | 27.928 | 36.636 | 74.095 | 1.00 23.01 | AAAA |
| MOTA | 2235 | 0 | λSN | 280 | 28.510 | 36.062 | 75.016 | 1.00 21.91 | AAAA |
| MOTA | 2236 | N | ILE | 281 | 26.711 | 36.300 | 73.689 | 1.00 18.74 | AAAA |
| MOTA | 2237 | CA | ILE | 281 | 26.005 | 35.179 | 74.294 | 1.00 18.74 | AAAA AAAA |
| MOTA | 2238 | CB | ILE | 281 | 24.566 | 35.067 | 73.758 | 1.00 19.31 | AAAA |
| MOTA | 2239 | CG2 | ILE | 281 | 23.977 | 33.725 | 74.135 | 1.00 28.87 | AAAA |
| ATOM | 2240 | | ILE | 281 | 23.710 | 36.206 | 74.308 | 1.00 23.51 | AAAA |
| MOTA | 2241 | CD1 | ILE | 281 | 22.279 | 36.193 | 73.776 | 1.00 26.47 | AAAA |
| MOTA | 2242 | С | ILE | 281 | 26.743 | 33.876 | 73.965 | 1.00 18.54 | AAAA |
| MOTA | 2243 | 0 | ILE | 281 | 26.830 | 32.973 | 74.801 | 1.00 19.69 | AAAA |
| MOTA | 2244 | N | VAL | 282 | | 33.765 | 72.744 | 1.00 17.72 | AAAA |
| | | | | | | | | | |

| | | ~ | 1727 | 282 | 27.976 | 32.553 | 72.352 | 1.00 14.89 | AAAA |
|--------------|--------------|------------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 2245 | | VAL | 282 | 28.359 | 32.565 | 70.852 | 1.00 18.50 | AAAA |
| MOTA | 2246 | CB | VAL | | 29.342 | 31.440 | 70.567 | 1.00 20.73 | AAAA |
| MOTA | 2247 | CG1 | | 282 282 | 27.105 | 32.363 | 69.994 | 1.00 17.49 | AAAA |
| MOTA | 2248 | CG2 | | 282 | 29.241 | 32.433 | 73.198 | 1.00 21.79 | AAAA |
| MOTA | 2249 | C | VAL | 282 | 29.568 | 31.360 | 73.715 | 1.00 25.80 | AAAA |
| MOTA | 2250 | 0 | VAL | 283 | 29.935 | 33.549 | 73.361 | 1.00 19.14 | AAAA |
| MOTA | 2251 | N | ARG | 283 | 31.161 | 33.548 | 74.150 | 1.00 23.51 | AAAA |
| MOTA | 2252. | CA | ARG | | 31.851 | 34.898 | 74.023 | 1.00 20.64 | AAAA |
| MOTA | 2253 | CB | ARG | 283 | 32.338 | 35.200 | 72.607 | 1.00 19.65 | AAAA |
| MOTA | 2254 | CG | ARG | 283 | 32.754 | 36.645 | 72.474 | 1.00 25.70 | AAAA |
| MOTA | 2255 | CD | ARG | 283 283 | 33.970 | 36.944 | 73.215 | 1.00 36.05 | AAAA |
| MOTA | 2256 | NE | ARG | 283 | 34.277 | 38.147 | 73.681 | 1.00 34.61 | AAAA |
| MOTA | 2257 | CZ | ARG | 283 | 33.448 | 39.169 | 73.488 | 1.00 35.23 | AAAA |
| MOTA | 2258 | NH1 NH2 | | 283 | 35.419 | 38.332 | 74.326 | 1.00 29.30 | AAAA |
| MOTA | 2259 | | ARG | 283 | 30.911 | 33.219 | 75.622 | 1.00 25.44 | AAAA |
| ATOM | 2260 | C | ARG | 283 | 31.754 | 32.600 | 76.272 | 1.00 23.12 | AAAA |
| ATOM | 2261 | 0 | GLU | 284 | 29.765 | 33.632 | 76.151 | 1.00 26.79 | AAAA |
| MOTA | 2262 | N CA | GLU | 284 | 29.462 | 33.338 | 77.553 | 1.00 31.77 | AAAA |
| MOTA | 2263 | CB | GLU | 284 | 28.243 | 34.115 | 78.033 | 1.00 30.96 | AAAA |
| ATOM | 2264 | CG | GLU | 284 | 28.399 | 35.605 | 77.957 | 1.00 50.56 | AAAA |
| ATOM | 2265 2266 | CD | GLU | 284 | 27.137 | 36.320 | 78.365 | 1.00 63.75 | AAAA |
| MOTA | 2267 | | GLU | 284 | 26.085 | 36.067 | 7 7. 738 | 1.00 68.93 | AAAA |
| MOTA | 2268 | | GLU | 284 | 27.198 | 37.133 | 79.309 | 1.00 72.01 | AAAA |
| ATOM | 2269 | C | GLU | 284 | 29.181 | 31.862 | 77.733 | 1.00 31.57 | AAAA |
| MOTA | 2270 | ō | GLU | 284 | 29.410 | 31.310 | 78.803 | 1.00 33.08 | AAAA |
| ATOM ATOM | 2271 | N | VAL | 285 | 28.673 | 31.221 | 76.686 | 1.00 23.37 | AAAA |
| ATOM | 2272 | CA | VAL | 285 | 28.354 | 29.807 | 76.774 | 1.00 23.25 | AAAA |
| ATOM | 2273 | CB | VAL | 285 | 27.221 | 29.407 | 75.789 | 1.00 24.77 | AAAA |
| ATOM | 2274 | | VAL | 285 | 26.952 | 27.913 | 75.881 | 1.00 26.98 | AAAA AAAA |
| ATOM | 2275 | CG2 | VAL | 285 | 25.940 | 30.181 | 76.107 | 1.00 24.98 | AAAA |
| MOTA | 2276 | С | VAL | 285 | 29.567 | 28.942 | 76.479 | 1.00 31.41 1.00 25.34 | AAAA |
| ATOM | 2277 | 0 | VAL | 285 | 29.833 | 27.983 | 77.195 | 1.00 25.34 | AAAA |
| ATOM | 2278 | N | PHE | 286 | 30.316 | 29.276 | . 75.431 | 1.00 27.27 | AAAA |
| ATOM | 2279 | CA | PHE | 286 | 31.463 | 28.457 | 75.086 73.667 | 1.00 22.26 | AAAA |
| ATOM | 2280 | CB | PHE | 286 | 31.289 | 27.904 | 73.536 | 1.00 25.71 | AAAA |
| ATOM | 2281 | CG | PHE | 286 | 30.168 | 26.918 27.274 | 72.917 | 1.00 22.88 | AAAA |
| ATOM | 2282 | | PHE | 286 | 28.971 | 25.631 | 74.069 | 1.00 24.49 | AAAA |
| ATOM | 2283 | | PHE | 286 | 30.294 27.919 | 26.365 | 72.829 | 1.00 19.85 | AAAA |
| ATOM | . 2284 | | PHE | 286 | 29.246 | 24.714 | 73.987 | 1.00 27.48 | AAAA |
| ATOM | 2285 | | PHE | 286 | 28.056 | 25.081 | 73.367 | 1.00 24.59 | AAAA |
| ATOM | 2286 | CZ | PHE | 286 286 | 32.854 | 29.059 | 75.225 | 1.00 21.53 | AAAA |
| MOTA | 2287 | C | PHE | 286 | 33.849 | 28.417 | 74.873 | 1.00 27.12 | AAAA |
| MOTA | 2288 | 0 | PHE GLY | 287 | 32.937 | 30.272 | 75.754 | 1.00 23.76 | AAAA |
| ATOM | 2289 | N CA | GLY | 287 | 34.237 | 30.896 | 75 901 | 1.00 24.17 | AAAA |
| ATOM | 2290 | C | GLY | 287 | 34.705 | 31.419 | 74.562 | 1.00 27.05 | AAAA |
| ATOM | 2291 2292 | ō | GLY | 287 | 33.888 | 31.670 | • 73 . 667 | 1.00 18.06 | AAAA |
| ATOM | 2293 | N | GLU | 288 | 36.017 | 31.576 | 74.414 | 1.00 23.21 | AAAA |
| MOTA MOTA | 2294 | CA | GLU | 288 | 36.583 | 32.085 | | 1.00 24.87 | AAAA |
| ATOM | 2295 | CB | GLU | 288 | 37.968 | 32.682 | 73.410 | 1.00 29.25 | AAAA AAAA |
| ATOM | 2296 | CG | GLU | 288 | 37.984 | 33.933 | 74.291 | 1.00 42.63 | AAAA |
| ATOM | 2297 | CD | GLU | 288 | 37.114 | 35.052 | 73.745 | 1.00 43.77 | AAAA |
| ATOM | 2298 | | GLU | 288 | 37.235 | 35.380 | 72.544 | 1.00 36.82 | AAAA |
| ATOM | 2299 | | GLU | 288 | 36.317 | 35.617 | 74.521 | 1.00 51.56 | AAAA |
| MOTA | 2300 | С | GLU | 288 | 36.693 | 31.028 | | 1.00 20.85 | AAAA |
| ATOM | 2301 | ō | GLU | 288 | 36.995 | 29.856 | 72.332 | 1.00 18.10 | AAAA |
| ATOM | 2302 | N | GLY | 289 | 36.447 | 31.468 | | 1.00 26.12 1.00 20.71 | AAAA |
| ATOM | 2303 | CA | GLY | 289 | 36.517 | 30.588 | | | AAAA |
| ATOM | 2304 | C | GLY | 289 | 37.126 | 31.318 | | | AAAA |
| ATOM | 2305 | 0 | GLY | 289 | 37.669 | 32.404 | | | AAAA |
| ATOM | 2306 | N | VAL | 290 | 37.032 | 30.724 | | | AAAA |
| MOTA | 2307 | CA | VAL | 290 | 37.572 | 31.312 | | | AAAA |
| MOTA | 2308 | CB | VAL | 290 | 38.150 | 30.192 | | | AAAA |
| ATOM | 2309 | | VAL | 290 | 38.667 | 30.769 | | | AAAA |
| 3 COM | 2310 | CG2 | VAL | 290 | 39.296 | 29.483 | . 03.320 | 1.00 20.10 | |

| ATOM | i 23: | 11 (| . VA | L 290 | 36.40 | 08 32.0 | 40 65.42 | 7 1 0 | | |
|--------------|---------------|------|----------------|--------------------|------------------|------------------|--------------------|------------------|--------------------|----------------|
| ATOM | | | - | | 35.3 | | | _ | 0 20.90 0 19.33 | AAAA |
| ATOM ATOM | | | | | 36.59 | 98 33.3 | | | 15.37 | AAAA AAAA |
| ATOM | | | A TY: B TY: | | 35.54 | | | 4 1.00 | 16.79 | AAAA |
| ATOM | | _ | B TY G TY | | 35.41 | | | 7 1.00 | 16.42 | AAAA |
| ATOM | | | D1 TY | | 35.37 36.36 | _ | | | 18.60 | AAAA |
| MOTA | | | El TY | | 36.36 | | 88 67.65 | | 21.77 | AAAA |
| ATOM | 231 | | D2 TY | | 34.38 | | | | 22.55 | AAAA |
| MOTA | | | E2 TYP | | 34.38 | | | | 17.34 | AAAA |
| ATOM | | _ | | 291 | - 35.36 | | | | 25.85 | AAAA |
| ATOM | | | | | 35.33 | 8 34.24 | | | 25.57 | AAAA . AAAA |
| MOTA MOTA | | | | | 35.72 | | | | 14.97 | AAAA |
| ATOM | | | TYF | | 36.77 | | | 1.00 | 15.21 | AAAA |
| ATOM | | | | | 34.66 | | | | 14.06 | AAAA |
| ATOM | 232 | | | | 34.67 34.46 | | | | 15.03 | AAAA |
| ATOM | 232 | | | | 35.34 | | | | 13.66 | AAAA |
| MOTA | 232 | 9 CI | 1 LEU | | 34.90 | | | | 19.04 | AAAA |
| ATOM | 2330 | | 2 LEU | 292 | 36.79 | | | | 15.17 19.18 | AAAA |
| ATOM | 233: | | LEU | | 33.56 | 4 35.32 | | | 16.62 | AAAA |
| ATOM | 2332 | | LEU | | 32.57 | | 8 61.107 | | 14.76 | AAAA AAAA |
| MOTA MOTA | 2333 2334 | | GLY | 293 | 33.72 | | | 1.00 | 18.62 | AAAA |
| ATOM | 2335 | | GLY GLY | 293 293 | 32.69 | | | 1.00 | 17.10 | AAAA |
| ATOM | 2336 | | GLY | 293 | 31.613 31.403 | | | | 23.44 | AAAA |
| ATOM | 2337 | | GLY | 294 | 30.915 | | | | 23.60 | AAAA |
| ATOM | 2338 | | GLY | 294 | 29.871 | | 37.083 8 56.434 | | 24.96 27.07 | AAAA |
| ATOM | 2339 | | GLY | 294 | 29.132 | 36.63 | | | 28.41 | AAAA AAAA |
| MOTA MOTA | 2340 2341 | | GLY | 294 | 29.605 | | | 1.00 | 25.66 | AAAA |
| ATOM | 2342 | | GLY. | 295 | 27.972 | | | | 20.33 | AAAA |
| ATOM | 2343 | C | GLY | 295 295 | 27.164 26.742 | | | | 20.14 | AAAA |
| ATOM | 2344 | ,õ | GLY | 295 | 26.550 | | 54.730 55.942 | | 25.34 | AAAA |
| MOTA | 2345 | N | GLY | 296 | 26.614 | 39.274 | | | 28.89 28.52 | AAAA |
| MOTA | 2346 | CA | GLY | 296 | 26.230 | | | | 23.21 | AAAA AAAA |
| MOTA MOTA | 2347 | C | GLY | 296 | 26.314 | | 53.059 | | 26.34 | AAAA |
| MOTA | 2348 2349 | N | GLY TYR | 296 | 27.359 | | | | 26.05 | AAAA |
| ATOM | 2350 | CA | TYR | 297 297 | 25.235 25.228 | | | | 22.61 | AAAA |
| ATOM | 2351 | CB | TYR | 297 | 24.265 | 42.644 41.861 | | | 22.58 | AAAA |
| MOTA | 2352 | CG | TYR | 297 | 24.502 | 40.352 | | | 23.68 | AAAA |
| MOTA | 2353 | | TYR | 297 | 23.981 | 39.571 | | 1.00 1.00 | | AAAA |
| ATOM | 2354 | | TYR | 297 | 24.269 | 38.196 | | 1.00 | | AAAA AAAA |
| ATOM ATOM | 2355 2: 36 | CD2 | | 297 | 25.307 | 39.725 | 49.577 | 1.00 | | AAAA |
| ATOM | 2.57 | CE2 | TYR TYR | 29 7 297 | 25.598 | 38.362 | 49.664 | 1.00 | 27.09 | AAAA |
| ATOM | 2538 | ОН | TYR | 297 | 25.085 25.407 | 37.606 36.261 | 50.696 | 1.00 | | AAAA |
| ATOM | 2359 | С | TYR | 297 | 24.916 | 44.138 | 50.739 51.320 | 1.00 | | AAAA |
| MOTA | 2360 | 0 | TYR | 297 | 24.841 | 44.714 | 50.237 | 1.00 | | AAAA |
| MOTA | 2361 | N. | HIS | 298 | 24.740 | 44.752 | 52.491 | 1.00 2 | | AAAA AAAA |
| ATOM | 2362 | | HIS | 298 | 24.480 | 46.188 | 52.591 | 1.00 2 | | AAAA |
| ATOM ATOM | 2363 2364 | CG . | HIS | 298 | 23.325 | 46.494 | 53.536 | 1.00 2 | 23.37 | AAAA |
| ATOM | 2365 | CD2 | HIS | 298 298 | 22.956 23.491 | 47.945 | 53.551 | 1.00 3 | | AAAA |
| ATOM | 2366 | ND1 | | 298 | 22.011 | 48.983 48.487 | 54.232 | 1.00 2 | | AAAA |
| ATOM | 2367 | CE1 | HIS | 298 | 21.978 | 49.797 | 52.707 52.868 | 1.00 3 | | AAAA |
| ATOM | 2368 | NE2 | HIS | 298 | 22.867 | 50.125 | 53.788 | 1.00 2 1.00 3 | | AAAA |
| MOTA | 2369 | С | HIS | 298 | 25.757 | 46.775 | 53.184 | 1.00 2 | | AAAA AAAA |
| ATOM | 2370 | | HIS | 298 | 26.135 | 46.439 | 54.306 | 1.00 2 | - | AAAA |
| atom atom | 2371 2372 | | PRO | 299 | 26.430 | 47.673 | 52.445 | 1.00 2 | | AAAA |
| ATOM ATOM | 2372 | | PRO | 299 | 26.078 | 48.207 | 51.117 | 1.00 2 | | AAAA |
| | 2374 | CB. | PRO PRO | 299 299 | 27.676 28.041 | 48.286 | 52,910 | 1.00 2 | | AAAA |
| ATOM | | | PRO | 299 | 26.678 | 49.228 49.600 | 51.755 | 1.00 2 | | AAAA |
| MOTA | | | PRO | 299 | 27.644 | 49.600 | 51.196 54.262 | 1.00 3 | | AAAA |
| • | | | - | · | | -0.331 | 74.505 | 1.00 2 | J./5 | AAAA |

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| | | | - | | 20 565 | 40 045 | 55.068 | 1.00 24.36 | AAAA |
|------|-------|-----|----------|-------|-----------|------------------|--------|------------|--------|
| MOTA | 2377 | 0 | PRO | 299 | 28.565 | 48.845 49.769 | 54.504 | 1.00 24.48 | AAAA |
| MOTA | 2378 | N | TYR | 300 | 26.602 | | 55.766 | 1.00 22.94 | AAAA |
| MOTA | 2379 | CA | TYR | 300 | 26.495 | 50.478 | 55.734 | 1.00 25.24 | AAAA |
| ATOM | 2380 | | TYR | 300 | 25.317 | 51.442 | 54.762 | 1.00 30.44 | AAAA |
| MOTA | 2381 | CG | TYR | 300 | 25.411 | 52.599 | 53.746 | 1.00 26.01 | AAAA |
| ATOM | 2382 | CD1 | | 300 | 26.366 | 52.634 | | 1.00 20.01 | AAAA |
| MOTA | 2383 | CE1 | TYR | 300 | 26.389 | 53.676 | 52.819 | 1.00 23.00 | 'AAAA |
| MOTA | 2384 | CD2 | TYR | 300 | 24.490 | 53.640 | 54.827 | 1.00 35.88 | AAAA |
| MOTA | 23.85 | CE2 | TYR | 300 | 24.501 | 54.677 | 53.916 | 1.00 38.44 | AAAA |
| ATOM | 2386 | CZ. | TYR | 300 | 25.448 | 54.689 | 52.913 | 1.00 33.41 | AAAA |
| MOTA | 2387 | OH | TYR | 300 | 25.417 | 55.700 | 51.990 | 1.00 33.41 | AAAA |
| ATOM | 2388 | С | TYR | 300 | 26.280 | 49.515 | 56.921 | 1.00 22.80 | AAAA |
| MOTA | 2389 | 0 | TYR | 300 - | 26.895 | 49.643 | 57.983 | | AAAA |
| ATOM | 2390 | N | ALA | 301 | 25.374 | 48.568 | 56.705 | 1.00 23.08 | AAAA |
| ATOM | 2391 | CA | ALA | 301 | 25.009 | 47.589 | 57.719 | 1.00 21.68 | - AAAA |
| ATOM | 2392 | CB | ALA | 301 | 23.893 | 46.687 | 57.198 | 1.00 19.52 | AAAA |
| MOTA | 2393 | С | ALA | 301 | 26.216 | 46.762 | 58.098 | 1.00 23.49 | |
| ATOM | 2394 | 0 | ALA | 301 | 26.507 | 46.570 | 59.274 | 1.00 21.21 | AAAA |
| ATOM | 2395 | N | LEU | 302 | 26.904 | 46.275 | 57.072 | 1.00 23.19 | AAAA |
| ATOM | 2396 | CA | LEU | 302 | 28.090 | 45.463 | 57.234 | 1.00 20.66 | AAAA |
| MOTA | 2397 | СВ | LEU | . 302 | 28.602 | 45.057 | 55.844 | 1.00 23.31 | AAAA |
| ATOM | 2398 | CG | LEU | 302 | 29.932 | 44.335 | 55.611 | 1.00 36.66 | AAAA |
| MOTA | 2399 | CD1 | | 302 | 29.979 | 43.849 | 54.170 | 1.00 38.41 | AAAA |
| ATOM | 2400 | | LEU | 302 | 31.104 | 45.255 | 55.879 | 1.00 28.52 | AAAA |
| MOTA | 2401 | c | LEU | 302 | 29.165 | 46.204 | 58.012 | 1.00 22.08 | AAAA |
| ATOM | 2402 | ō | LEU | 302 | 29.653 | 45.713 | 59.020 | 1.00 20.43 | AAAA |
| ATOM | 2403 | Ŋ | ALA | 303 | 29.517 | 47.401 | 57.549 | 1.00 19.58 | AAAA |
| ATOM | 2404 | CA | ALA | 303 | 30.567 | 48.173 | 58.197 | 1.00 19.77 | AAAA |
| ATOM | 2405 | CB | ALA | 303 | 30.816 | 49.460 | 57.432 | 1.00 21.69 | AAAA |
| MOTA | 2406 | C | ALA | 303 | 30.324 | 48.485 | 59.657 | 1.00 19.19 | AAAA |
| | 2407 | ō | ALA | 303 | 31.216 | 48.310 | 60.489 | 1.00 22.51 | AAAA |
| ATOM | 2408 | Ŋ | ARG | 304 | 29.128 | 48.954 | 59.993 | 1.00 20.12 | AAAA |
| MOTA | 2409 | CA | ARG | 304 | 28.872 | 49.296 | 61.377 | 1.00 18.04 | AAAA |
| MOTA | 2410 | CB | ARG | 304 - | 27.566 | 50.114 | 61.511 | 1.00 21.09 | AAAA |
| MOTA | 2411 | CG | ARG | 304 | 27.532 | 51.481 | 60.792 | 1.00 24.34 | AAAA |
| ATOM | 2412 | CD | ARG | 304 | 26.259 | 52.259 | 61.206 | 1.00 27.09 | AAAA |
| ATOM | 2413 | NE | ARG | 304 | 25.090 | 51.398 | 61.116 | 1.00 45.73 | AAAA |
| MOTA | 2414 | CZ | ARG | 304 | 23.965 | 51.549 | 61.808 | 1.00 39.82 | AAAA |
| MOTA | 2415 | | ARG | 304 | 23.813 | 52.550 | 62.677 | 1.00 28.40 | AAAA |
| ATOM | 2416 | | ARG | 304 | 22.991 | 50.667 | 61.647 | 1.00 41.77 | AAAA |
| ATOM | 2417 | С | ARG | 304 | 28.794 | 48.073 | 62.280 | 1.00 21.00 | AAAA |
| ATOM | 2418 | ò | ARG | 304 | 29.313 | 48.087 | 63.397 | 1.00 19.45 | AAAA |
| MOTA | 2419 | N | ALA | 305 | 28.159 | 47.008 | 61.796 | 1.00 19.93 | AAAA |
| MOTA | 2420 | CA | ALA | 305 | 28.002 | 45.809 | 62.610 | 1.00 18.70 | AAAA |
| MOTA | 2421 | CB | ALA | 305 | 26.998 | 44.830 | 61.933 | 1.00 18.26 | AAAA · |
| MOTA | 2422 | C | ALA | 305 | 29.311 | 45.109 | 62.915 | 1.00 16.46 | AAAA |
| ATOM | 2423 | ō | ALA | 305 | 29.564 | 44.736 | 64.061 | 1.00 .9.49 | AAAA |
| ATOM | 2424 | N | TRP | 306 | 30.152 | 44.909 | 61.905 | 1.00 1.92 | AAAA |
| MOTA | 2425 | CA | TRP | 306 | 31.423 | 44.268 | 62.183 | 1.00 18.99 | AAAA |
| ATOM | 2426 | CB | TRP | 306 | 32.151 | 43.865 | 60.902 | 1.00 17.96 | AAAA |
| ATOM | 2427 | CG | TRP | 306 | 31.632 | 42.564 | 60.333 | 1.00 21.34 | AAAA |
| ATOM | 2428 | | TRP | 306 | 31.852 | 42.058 | 59.014 | 1.00 16.55 | AAAA |
| ATOM | 2429 | | TRP | 306 | 31.243 | 40.785 | 58.949 | 1.00 19.37 | AAAA |
| MOTA | 2430 | | TRP | 306 | 32.507 | 42.556 | 57.878 | 1.00 17.80 | AAAA |
| MOTA | 2431 | CD1 | TRP | 306 | 30.919 | 41.610 | 60.995 | 1.00 19.88 | AAAA |
| ATOM | 2432 | NE1 | TRP | 306 | 30.680 | 40.535 | 60.170 | 1.00 15.95 | AAAA |
| MOTA | | | TRP | 306 | 31.270 | 40.002 | 57.787 | 1.00 24.85 | AAAA |
| MOTA | 2433 | C73 | TRP | 306 | 32.534 | 41.781 | 56.725 | 1.00 29.69 | AAAA |
| MOTA | 2434 | C#3 | TRP | 306 · | 31.917 | 40.513 | 56.691 | 1.00 17.04 | AAAA |
| MOTA | 2435 | | TRP | 306 | 32.289 | 45.188 | 63.018 | 1.00 20.26 | AAAA |
| MOTA | 2436 | C | | 306 | 33.159 | 44.726 | 63.752 | 1.00 21.20 | AAAA |
| ATOM | 2437 | 0 | TRP | 307 | 32.061 | 46.491 | | 1.00 18.60 | AAAA |
| ATOM | 2438 | N | THR | 307 | 32.843 | 47.412 | 63.722 | 1.00 16.88 | AAAA |
| ATOM | 2439 | CA | | 307 | 32.579 | 48.885 | | 1.00 22.05 | AAAA |
| MOTA | | CB | THR | 307 | 33.218 | 49.132 | 054 | 1.00 21.58 | AAAA |
| MOTA | 2441 | OGI | THR | 307 | 33.126 | 49.857 | | | AAAA |
| ATOM | 2442 | (G2 | THR | 307 | ,,,,,,,,, | | | | • |
| | | • | | | | | | | |

| ATOM | 2443 | | THI | R 307 | 32.493 | 3 47.146 | 65.187 | 1.00 17.47 | AAAA |
|--------------|--------------|----------|-----------------|------------|------------------|------------------|------------------|--------------------------|----------------|
| ATOM | 2444 | _ | THI | | 33.377 | 7 47.142 | 66.039 | | AAAA |
| ATOM | 2445 | | LE | | 31.216 | | | 1.00 19.97 | AAAA |
| MOTA | 2446 | | | | 30.834 | | | | AAAA |
| MOTA | 2447 2448 | | | | 29.318 | | | | AAAA |
| ATOM ATOM | 2449 | | LEU 1 LEU | | 28.415 | | | | AAAA |
| ATOM | 2450 | | 2 LET | | 26.937 28.870 | | | 1.00 25.01 | AAAA |
| ATOM | 2451 | | LET | | 31.578 | | | | AAAA |
| ATOM | 2452 | | LEU | | 32.056 | | | | AAAA |
| ATOM | 2453 | | ILE | | 31.677 | | | 1.00 22.27 1.00 22.54 | AAAA |
| ATOM | 2454 | | | | 32.377 | | | 1.00 22,34 | AAAA AAAA |
| ATOM | 2455 | CB | ILE | 309 | 32.318 | | | 1.00 18.12 | AAAA |
| MOTA | 2456 | CG | 2 ILE | 309 | 33.170 | | | 1.00 24.16 | AAAA |
| ATOM | 2457 | | 1 ILE | | 30.871 | 41.655 | | 1.00 18.26 | AAAA |
| ATOM | 2458 | | 1. ILE | | 30.205 | 40.989 | 66.586 | 1.00 26.57 | AAAA |
| ATOM | 2459 | | ILE | | 33.849 | | | 1.00 20.84 | AAAA |
| ATOM | 2460 | | ILE | | 34.426 | | | 1.00 25.20 | AAAA |
| ATOM | 2461 | N | TRP | | 34.466 | | 66.214 | 1.00 16.86 | AAAA |
| ATOM | 2462 | .CA | TRP | | 35.888 | | | 1.00 17.86 | AAAA |
| ATOM ATOM | 2463 2464 | CB CG | TRP TRP | 310 310 | 36.439 | 45.319 | 65.235 | 1.00 14.83 | AAAA |
| ATOM | 2465 | | TRP | 310 | 37.879 38.967 | 45.648 44.718 | | 1.00 16.63 | AAAA |
| ATOM | 2466 | | 2 TRP | 310 | 40.131 | 45.478 | 65.560 65.799 | 1.00 18.62 1.00 25.60 | AAAA |
| ATOM | 2467 | CE. | | 310 | 39.069 | 43.319 | 65.529 | 1.00 25.60 | AAAA AAAA |
| ATOM | 2468 | CD: | TRP | 310 | 38.418 | 46.895 | 65.533 | 1.00 19.82 | AAAA |
| MOTA | 2469 | | l TRP | 310 | 39.768 | 46.801 | 65.777 | 1.00 25.84 | AAAA |
| MOTA | 2470 | CZ | | 310 | 41.383 | 44.887 | 66.006 | 1.00 26.14 | AAAA |
| ATOM | 2471 | CZ. | | 310 | 40.308 | 42.730 | 65.735 | 1.00 24.89 | AAAA |
| MOTA | 2472 | CH | | 310 | 41.452 | 43.515 | 65.971 | 1.00 24.96 | AAAA |
| MOTA MOTA | 2473 2474 | С 0 | TRP TRP | 310 | 36.112 | 45.263 | 67.733 | 1.00 20.86 | AAAA |
| ATOM | 2475 | N | CYS | 310 311 | 37.050 35.242 | 44.957 | 68.478 | 1.00 21.38 | AAAA |
| ATOM | 2476 | CA | CYS | 311 | 35.349 | 46.226 46.971 | 68.030 69.280 | 1.00 24.22 | AAAA |
| ATOM | 2477 | CB | CYS | 311 | 34.297 | 48.097 | 69.343 | 1.00 27.66 1.00 25.37 | AAAA AAAA |
| ATOM | 2478 | SG | CYS | 311 | 34.618 | 49.528 | 68.253 | 1.00 27.22 | AAAA |
| ATOM | 2479 | C | CYS | 311 | 35.224 | 46.042 | 70.490 | 1.00 22.95 | AAAA |
| ATOM | 2480 | 0 | CYS | 311 | 35.986 | 46.180 | 71.441 | 1.00 25.47 | AAAA |
| ATOM | 2481 | N | GLU | 312 | 34.284 | 45.089 | 70.457 | 1.00 17.03 | AAAA |
| MOTA | 2482 | CA | GLU | 312 | 34.120 | 44.129 | 71.569 | 1.00 22.44 | AAAA |
| MOTA MOTA | 2483 2484 | CB CG | GLU | 312 312 | 33.011 | 43.110 | 71.280 | 1.00 20.81 | AAAA |
| ATOM | 2485 | CD | GLU | 312 | 31.856 32.265 | 43.048 42.971 | 72.258 73.717 | 1.00 43.65 | AAAA |
| ATOM | 2486 | | GLU | 312 | 33.022 | 42.059 | 74.119 | 1.00 29.63 1.00 38.85 | AAAA AAAA |
| ATOM | 2487 | OE2 | | 312 | 31.804 | 43.844 | 74.473 | 1.00 53.22 | AAAA |
| ATOM | 2488 | С | GLI | 312 | 35.395 | 43.309 | 71.778 | 1.00 27.47 | AAAA |
| MOTA | 2489 | 0 | $G\Gamma\Gamma$ | 312 | 35.899 | 43.178 | 72:895 | 1.00 22.33 | AAAA |
| ATOM | 2490 | N | LEL | 313 | 35.899 | 42.723 | 70.696 | 1.00 23.82 | AAAA |
| MOTA | 2491 | CA | LEU | 313 | 37.101 | 41.889 | 70.771 | 1.00 20.72 | AAAA |
| ATOM | 2492 | CB CG | LEU | 313 | 37.380 | 41.222 | 69.422 | 1.00 27.82 | AAAA |
| ATOM ATOM | 2493 2494 | | LEU LEU | 313 313 | 36.403 36.839 | 40.167 | 68.903 | 1.00 33.55 | AAAA |
| ATOM | 2495 | | LEU | 313 | 36.379 | 39.738 38.981 | | 1.00 24.03 | AAAA |
| ATOM | 2496 | c | LEU | 313 | 38.343 | 42.670 | 69.846 71.181 | 1.00 28.20 1.00 18.21 | AAAA AAAA |
| ATOM | 2497 | ō | LEU | 313 | 39.119 | 42.205 | 72.017 | 1.00 21.48 | AAAA |
| MOTA | 2498 | N | SER | 314 | 38.492 | 43.848 | 70.580 | 1.00 19.41 | AAAA |
| ATOM | 2499 | CA | SER | 314 | 39.627 | 44.753 | 70.775 | 1.00 28.26 | AAAA |
| ATOM | 2500 | CB | SER | 314 | 39.625 | 45.821 | 69.663 | 1.00 22.55 | AAAA |
| MOTA | 2501 | OG | SER | 314 | 40.732 | 46.696 | 69.759 | 1.00 61.92 | AAAA |
| MOTA | 2502 | С | SER | 314 | 39.619 | 45.429 | 72.144 | 1.00 30.18 | AAAA |
| ATOM | 2503 | 0 | SER | 314 | 40.631 | 45.969 | 72.590 | 1.00 25.04 | AAAA |
| ATOM | 2504 | N | GLY | 315 | 38.477 | 45.407 | 72.806 | 1.00 28.04 | AAAA |
| MOTA MOTA | 2505 2506 | CA C | GLY GLY | 315 315 | 38.393 38.324 | 46.009 | 74.119 | 1.00 33.84 | AAAA |
| ATOM | | 0 | GLY | 315 | 38.811 | 47.518 48.178 | 74.105 75.022 | 1.00 36.93 | AAAA |
| MOTA | | N | ARG | 316 | 37.739 | 48.090 | 73.022 | 1.00 37.00 1.00 31.33 | ДДАД ДДДД . |
| | | | | | | -0.030 | | 1.00 31.33 | . ~~~~ |

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| n mon | 2509 | CA | ARG | 316 | 37.631 | 49.536 | 73.042 | 1.00 39.10 | AAAA |
|--------|------|-----------|-----|------|--------|--------|--------|------------|------|
| MOTA | 2510 | CB | ARG | 316 | 38.347 | 50.108 | 71.830 | 1.00 45.15 | AAAA |
| MOTA | 2511 | CG | ARG | 316 | 37.722 | 49.834 | 70.501 | 1.00 46.02 | AAAA |
| MOTA | 2512 | CD | ARG | 316 | 38.620 | 50.459 | 69.449 | 1.00 44.83 | AAAA |
| MOTA | 2512 | NE | ARG | 316 | 39.898 | 49.767 | 69.357 | 1.00 37.91 | AAAA |
| MOTA | | | ARG | 316 | 40.945 | 50.219 | 68.674 | 1.00 27.39 | AAAA |
| MOTA | 2514 | CZ NH1 | | 316 | 40.854 | 51.371 | 68.034 | 1.00 50.24 | AAAA |
| ATOM | 2515 | | | 316 | 42.054 | 49.493 | 68.572 | 1.00 34.51 | AAAA |
| MOTA | 2516 | NH2 | | 316 | 36.179 | 49.984 | 73.058 | 1.00 35.43 | AAAA |
| MOTA | 2517 | C | ARG | | 35.292 | 49.271 | 72.596 | 1.00 30.71 | AAAA |
| ATOM | 2518 | 0 | ARG | 316 | 35.232 | 51,162 | 73.612 | 1.00 34.06 | AAAA |
| MOTA | 2519 | N | GLU | 317 | 34.569 | 51.663 | 73.671 | 1.00 37.96 | AAAA |
| ATOM | 2520 | CA | GLU | 317 | 34.481 | 52.914 | 74.552 | 1.00 43.60 | AAAA |
| MOTA | 2521 | CB | GLU | 317 | 33.961 | 52.630 | 75.960 | 1.00 60.36 | AAAA |
| ATOM | 2522 | CG | GLU | 317 | 34.768 | 51.575 | 76.701 | 1.00 70.70 | AAAA |
| ATOM | 2523 | CD | GLU | 317 | | 51.217 | 77.832 | 1.00 76.71 | AAAA |
| MOTA | 2524 | | GLU | 317 | 34.375 | 51.104 | 76.162 | 1.00 78.36 | AAAA |
| ATOM | 2525 | | GLU | 317 | 35.793 | | 72.280 | 1.00 75.55 | AAAA |
| MOTA | 2526 | С | GLU | 317 | 34.068 | 51.958 | 71.390 | 1.00 33.03 | AAAA |
| ATOM | 2527 | 0 | GLU | 317 | 34.843 | 52.322 | | 1.00 32.51 | AAAA |
| ATOM | 2528 | N | VAL | 318 | 32.767 | 51.772 | 72.094 | 1.00 30.32 | AAAA |
| MOTA | 2529 | CA | VAL | 318 | 32.138 | 52.012 | 70.808 | | AAAA |
| MOTA | 2530 | CB | VAL | 318 | 30.877 | 51.138 | 70.638 | 1.00 36.48 | |
| ATOM | 2531 | CG1 | VAL | 318 | 30.278 | 51.366 | 69.268 | 1.00 40.43 | AAAA |
| ATOM | 2532 | CG2 | VAL | 318 | 31.222 | 49.674 | 70.846 | 1.00 33.75 | AAAA |
| ATOM | 2533 | С | VAL | 318 | 31.719 | 53.465 | 70.737 | 1.00 28.96 | AAAA |
| MOTA | 2534 | 0 | VAL | 318 | 30.930 | 53.915 | 71.556 | 1.00 33.56 | AAAA |
| ATOM | 2535 | N | PRO | 319 | 32.258 | 54.229 | 69.773 | 1.00 29.20 | AAAA |
| ATOM | 2536 | CD | PRO | 319 | 33.243 | 53.924 | 68.726 | 1.00 31.62 | AAAA |
| ATOM | 2537 | CA | PRO | 319 | 31.858 | 55.637 | 69.684 | 1.00 28.99 | AAAA |
| ATOM | 2538 | CB | PRO | 319 | 32.709 | 56.154 | 68.528 | 1.00 32.17 | AAAA |
| ATOM | 2539 | CG | PRO | 319 | 32.850 | 54.926 | 67.664 | 1.00 41.36 | AAAA |
| ATOM | 2540 | С | PRO | 319 | 30.365 | 55.680 | 69.377 | 1.00 36.95 | AAAA |
| ATOM | 2541 | 0 | PRO | 319 | 29.847 | 54.795 | 68.695 | 1.00 32.86 | AAAA |
| ATOM | 2542 | N | GLU | 320 | 29.646 | 56.683 | 69.855 | 1.00 34.61 | AAAA |
| ATOM | 2543 | CA | GLU | 320 | 28.230 | 56.657 | 69.544 | 1.00 35.13 | AAAA |
| ATOM | 2544 | CB | GLU | 320 | 27.419 | 57.416 | 70.595 | 1.00 52.97 | AAAA |
| ATOM | 2545 | CG | GLU | 320 | 27.751 | 58.875 | 70.738 | 1.00 56.06 | AAAA |
| ATOM | 2546 | CD | GLU | 320 | 26.822 | 59.558 | 71.721 | 1.00 65.58 | AAAA |
| ATOM | 2547 | | GLU | 320 | 25.604 | 59.619 | 71.444 | 1.00 64.27 | AAAA |
| ATOM | 2548 | | GLU | 320 | 27.306 | 60.022 | 72.775 | 1.00 72.99 | AAA |
| ATOM | 2549 | C | GLU | 320 | 27.943 | 57.192 | 68.153 | 1.00 35.13 | AAAA |
| ATOM | 2550 | 0 | GLU | 320 | 26.916 | 56.879 | 67.565 | 1.00 37.43 | AAAA |
| ATOM | 2551 | N | LYS | 321 | 28.880 | 57.953 | 67.604 | 1.00 28.22 | AAAA |
| ATOM | 2552 | CA | LYS | 321 | 28.700 | 58.555 | 66.289 | 1.00 36.58 | AAAA |
| ATOM | 2553 | CB | LYS | 321 | 28.666 | 60.071 | 66.454 | 1.00 44.87 | AAAA |
| ATOM | 2554 | CG | LYS | 321 | 29.987 | 60.606 | 67.023 | 1.00 55.73 | AAA" |
| ATOM | 2555 | CD | LYS | 321 | 30.305 | 60.020 | 68.410 | 1.00 57.27 | AAA |
| ATOM | 2556 | CE | LYS | 321 | 31.733 | 60.310 | 68.840 | 1.00 54.59 | AAA |
| ATOM | 2557 | NZ | LYS | 321 | 32.024 | 61.774 | 68.848 | 1.00 67.47 | AAAA |
| ATOM | 2558 | С | LYS | 321 | 29.823 | 58.211 | 65.315 | 1.00 34.44 | AAAA |
| ATOM | 2559 | ō | LYS | 321 | 30.912 | 57.818 | 65.731 | 1.00 33.83 | AAAA |
| ATOM | 2560 | N | LEU | 322 | 29.549 | 58.354 | 64.019 | 1.00 30.21 | AAAA |
| MOTA | 2561 | CA | LEU | 322 | 30.575 | 58.135 | 62.998 | 1.00 29.45 | AAAA |
| ATOM | 2562 | CB | LEU | 322 | 29.966 | 57.677 | 61.677 | 1.00 32.21 | AAAA |
| ATOM | 2563 | CG | LEU | 322 | 29.240 | 56.338 | 61.651 | 1.00 38.94 | AAAA |
| ATOM | 2564 | | LEU | 3:22 | 29.008 | 55.977 | 60.186 | 1.00 38.44 | AAAA |
| ATOM | 2565 | | LEU | 322 | 30.072 | 55.261 | 62.337 | 1.00 42.11 | AAAA |
| | 2566 | C | LEU | 322 | 31.228 | 59.503 | 62.783 | 1.00 33.28 | AAAA |
| MOTA | 2567 | õ | LEU | 322 | 30.544 | 60.519 | 62.872 | 1.00 31.45 | AAAA |
| MOTA | 2568 | N | ASN | 323 | 32.533 | 59.539 | 62.519 | 1.00 34.38 | AAAA |
| MOTA | 2569 | CA | ASN | 323 | 33.208 | 60.824 | 62.294 | 1.00 36.53 | AAAA |
| ATOM | | CB | ASN | 323 | 34.701 | 60.737 | 62.600 | 1.00 42.85 | AAAA |
| ATOM | 2570 | CG | ASN | 323 | 35.484 | 60.081 | 61.480 | 1.00 50.51 | AAAA |
| ATOM | 2571 | | ASN | 323 | 35,215 | 58.942 | 61.109 | 1.00 51.23 | AAAA |
| ATOM | 2572 | | ASN | 323 | 36.455 | 60.807 | 60.928 | 1.00 60.23 | AAAA |
| ATOM . | | | ASN | 323 | 33.027 | 61.171 | 60.822 | 1.00 34.69 | AAAA |
| MOTA | 2574 | ,C | | | | | • | | • |
| - | | | | | | | | | |

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| ATOM | 257 | 5 0 | ASN | 323 | 32.4 | 29 60.39 | 5 60.075 | 1.00 34.06 | 3333 |
|--------------|---------------|----------|------------|---------------------|------------------|----------|------------------|--------------------------|--------------|
| ATOM | 257 | 6 N | ASN | | 33.5 | | _ | | AAAA |
| ATOM | 257 | 7 C2 | A ASN | | 33.3 | | | | AAAA |
| ATOM | 257 | 8 CE | | | 33.8 | | | | AAAA |
| ATOM | 257 | 9 CG | | | 32.9 | | | | AAAA |
| ATOM | 258 | O OI | Ol ASN | | 31.7 | | | | AAAA |
| MOTA | 258 | | 2 ASN | | 33.5 | | | | AAAA |
| ATOM | 2582 | | ASN | | 34.0 | | | | AAAA |
| ATOM | 2583 | | ASN | | 33.4 | | | | AAAA |
| ATOM | 2584 | | LYS | | 35.2 | | | | AAAA |
| MOTA | 2585 | | | | - 35.9 | | | | AAAA |
| MOTA | 2586 | | | | 37.3 | | | | AAAA |
| ATOM | 2587 | | | | 38.2 | | | | AAAA |
| MOTA | 2588 | | | | 39.6 | | | | AAAA |
| ATOM | 2589 | | | | 40.1 | | | | AAAA |
| ATOM | 2590 | | | | 41.6 | | | | AAAA |
| ATOM | 2591 | | LYS | | 35.10 | | | | AAAA |
| ATOM | 2592 | | LYS | 325 | 35.0 | | | 1.00 27.99 1.00 31.80 | AAAA |
| MOTA | 2593 | | ALA | 326 | 34.60 | | | | AAAA |
| ATOM | 2594 | | ALA | 326 | 33.78 | | | 1.00 26.07 1.00 24.38 | AAAA |
| MOTA | 2595 | | ALA | 326 | 33.47 | | | 1.00 27.34 | AAAA |
| MOTA | 2596 | С | ALA | 326 | 32.47 | | | 1.00 27.34 | AAAA |
| MOTA | 2597 | 0 | λLÁ | 326 | 32.13 | | | 1.00 23.78 | AAAA |
| ATOM | 2598 | N | LYS | 327 | 31.74 | | | 1.00 27.31 | AAAA AAAA |
| ATOM | 2599 | CA | LYS | 327 | 30.50 | | | 1.00 28.56 | AAAA |
| MOTA | 2600 | CB | LYS | 327 | 29.75 | | | 1.00 28.87 | AAAA |
| MOTA | 2601 | CG | LYS | 327 | 29.49 | | | 1.00 36.72 | AAAA |
| ATOM | 2602 | CD | LYS | 327 | · 28.64 | | | 1.00 40.34 | AAAA |
| ATOM | 2603 | CE | LYS | 327 | 28.64 | | 60.769 | 1.00 38.91 | AAAA |
| ATOM- | 2604 | NZ | LYS | 327 | 28.16 | 3 60.429 | 61.556 | 1.00 47.67 | AAAA |
| MOTA | 2605 | С | LYS | - | 30.79 | | 55.269 | 1.00 29.15 | AAAA |
| MOTA | 2606 | 0 | LYS | 327 | 30.09 | 7 58.719 | 54.393 | 1.00 27.76 | AAAA |
| ATOM | 2607 | N | GLU | 328 | 31.82 | 9 60.015 | 54.972 | 1.00 31.59 | AAAA |
| ATOM | 2608 | CA | GLU | 32 <mark>.</mark> 8 | 32.16 | | 53.581 | 1.00 28.93 | AAAA |
| MOTA | 2609 | CB | GLU | 328 | 33.25 | | 53.515 | 1.00 32.30 | AAAA |
| ATOM | 2610 | CG | GLU | 328 | 32.74 | | 54.067 | 1.00 47.50 | AAAA |
| ATOM | 2611 | CD | GLU | 328 | 33.76 | _ | 54.032 | 1.00 46.67 | AAAA |
| ATOM | 2612 | OE1 | | 328 | 34.32 | | 52.951 | 1.00 56.88 | AAAA |
| ATOM | 2613 | OE2 | | 328 | 33.98 | | 55.087 | 1.00 42.24 | AAAA |
| ATOM ATOM | .2614 2615 | С | GLU | 328 | 32.57 | | 52.871 | 1.00 30.46 | AAAA |
| ATOM | 2616 | И | GLU LEU | 328 | 32.22 | | 51.704 | 1.00 26.29 | AAAA |
| MOTA | 2617 | CA | LEU | 329 329 | 33.29 | | 53.584 | 1.00 24.93 | AAAA |
| ATOM | 2618 | CB | LEU | 329 | 33.70 | | 53.017 | 1.00 24.80 | AAAA |
| MOTA | 2619 | CG | LEU | 329 | 34.478 34.736 | | 54.053 | 1.00 25.70 | AAAA |
| ATOM | 2620 | | LEU | 329 | 5.569 | | 53.703 | 1.00 19.71 | AAAA |
| ATOM | 2621 | | LEU | 329 | 55.412 | | 52.430 | 1.00 25.26 | AAAA |
| ATOM | 2622 | c | LEU | 329 | 2.443 | | 54.863 52.603 | 1.00 24.73 1.00 23.50 | AAAA |
| MOTA | 2623 | ō | LEU | 329 | 32.310 | | 51.453 | 1.00 25.60 | AAAA |
| ATOM | 2624 | N | LEU | 330 | 31.516 | | 53.539 | 1.00 23.00 | AAAA |
| ATOM | 2625 | CA | LEU | 330 | 30.289 | | 53.242 | 1.00 23.02 | AAAA |
| ATOM | 2626 | CB | LEU | 330 | 29.414 | | 54.484 | 1.00 21.74 | AAAA |
| ATOM | 2627 | CG | LEU | 330 | 30.039 | | 55.642 | 1.00 25.29 | AAAA AAAA |
| ATOM | 2628 | | LEU | 330 | 28.984 | | 56.724 | 1.00 30.58 | AAAA |
| ATOM | 2629 | | LEU | 330 | 30.538 | | 55.168 | 1.00 22.44 | AAAA |
| ATOM | 2630 | С | LEU | 330 | 29.491 | | 52.113 | 1.00 26.94 | AAAA |
| ATOM | 2631 | Ö | LEU | 330 | 28.968 | | 51.252 | 1.00 26.65 | AAAA |
| ATOM | 2632 | N | LYS | 331 | 29.404 | | 52.111 | 1.00 30.82 | AAAA |
| ATOM | 2633 | CA | LYS | 331 | 28.667 | | 51.066 | 1.00 29.53 | AAAA |
| ATOM | 2634 | CB | LYS | 331 | 28.537 | | 51.407 | 1.00 29.67 | AAAA |
| ATOM | 2635 | CG | LYS | 331 | 27.814 | | 52.714 | 1.00 36.06 | AAAA |
| ATOM | 2636 | CD | LYS | 331 | 27.688 | | 52.990 | 1.00 42.75 | AAAA |
| ATON | 2637 | CE | LYS | 331 | 26.828 | | 51.939 | 1.00 53.98 | AAAA |
| ATOM | 2638 | NZ | LYS | 331 | 26.634 | | 52.234 | 1.00 67.57 | AAAA |
| MOTA | 2639 | | LYS | 331 | 29.315 | | 49.692 | 1.00 30.07 | AAAA |
| MOTA | 2640 | 0 | LYS | 331 | 28.634 | 57.759 | 48.672 | 1.00 36.20 | AAAA |
| | | | | • | | | - | • • • • • • | |

| | | | | | 00.600 | C7 30E | 49.657 | 1.00 30.08 | AAAA |
|-------|------|-----|-----|-------|--------|---------|--------|--------------|--------|
| ATOM | 2641 | N | SER | 332 | 30.608 | 57.305 | | | |
| ATOM | 2642 | CA | SER | 332 | 31.322 | 57.153 | 48.385 | 1.00 33.35 | AAAA |
| ATOM | 2643 | CB | SER | .332 | 32.834 | 57.312 | 48.590 | 1.00 40.36 | AAAA |
| ATOM | 2644 | OG | SER | 332 | 33.396 | 56.169 | 49.219 | 1.00 34.04 | AAAA |
| | 2645 | C | SER | 332 | 31.061 | 55.821 | 47.693 | 1.00 37.72 | AAAA |
| MOTA | | ō | SER | 332 | 31.354 | 55.661 | 46.507 | 1.00 30.78 | AAAA |
| ATOM | 2646 | | | 333 | 30.521 | 54.865 | 48.440 | 1.00 30.61 | AAAA |
| MOTA | 2647 | N | ILE | | | 53.547 | 47.899 | 1.00 37.59 | AAAA |
| MOTA | 2648 | CA | ILE | 333 | 30.219 | | 49.022 | 1.00 33.59 | AAAA |
| MOTA | 2649 | CB | ILE | . 333 | 29.901 | 52.551 | | | AAAA |
| ATOM | 2650 | CG2 | ILE | 333 | 29.738 | 51.146 | 48.442 | 1.00 37.05 | |
| ATOM | 2651 | CG1 | ILE | 333 | 31.015 | 52.564 | 50.065 | 1.00 38.95 | AAAA |
| MOTA | 2652 | | ILE | . 333 | 30.706 | 51.727 | 51.282 | 1.00 46.83 | AAAA |
| | 2653 | C | ILE | 333 | 28.990 | 53.620 | 46.998 | 1.00 43.41 | AAAA |
| MOTA | | | ILE | 333 | 27.889 | 53.876 | 47.479 | 1.00 46.24 | AAAA |
| ATOM | 2654 | 0 | | 334 | 29.158 | 53.423 | 45.696 | 1.00 47.97 | AAAA |
| ATOM | 2655 | N | ASP | | 27.976 | 53.447 | 44.847 | 1.00 53.47 | - AAAA |
| ATOM | 2656 | CA | ASP | 334 | | | 43.358 | 1.00 61.52 | AAAA |
| MOTA | 2657 | CB | ASP | 334 | 28.333 | 53.535 | | 1.00 64.75 | AAAA |
| ATOM | 2658 | CG | ASP | 334 | 29.223 | 52.406 | 42.897 | | |
| ATOM | 2659 | op1 | ASP | 334 | 29.379 | 52.248 | 41.666 | 1.00 66.93 | AAAA |
| ATOM | 2660 | OD2 | ASP | 334 | 29.779 | 51.691 | 43.758 | 1.00 65.93 · | AAAA |
| | 2661 | c | ASP | 334 | 27.248 | 52.144 | 45.161 | 1.00 51.83 | AAAA |
| ATOM | 2662 | õ | ASP | 334 | 27.626 | 51.067 | 44.699 | 1.00 46.80 | AAAA |
| ATOM | | | | 335 | 26.215 | 52.249 | 45.986 | 1.00 54.96 | AAAA |
| MOTA | 2663 | N | PHE | | 25.455 | 51.080 | 46.392 | 1.00 50.60 | AAAA |
| ATOM | 2664 | CA | PHE | 335 | | 51.003 | 47.920 | 1.00 39.55 | AAAA |
| ATOM | 2665 | CB | PHE | 335 | 25.413 | | 48.440 | 1.00 37.98 | AAAA |
| ATOM | 2666 | CG | PHE | 335 | 24.380 | 50.054 | | 1.00 37.38 | AAAA |
| MOTA | 2667 | CD1 | PHE | 335 | 24.389 | 48.715 | 48.054 | | |
| ATOM | 2668 | CD2 | PHE | 335 | 23.362 | 50.506 | 49.262 | 1.00 34.23 | AAAA |
| ATOM | 2669 | CE1 | PHE | 335 | 23.389 | 47.842 | 48.478 | 1.00 49.80 | AAAA |
| ATOM | 2670 | CE2 | | 335 | 22.361 | 49.644 | 49.689 | 1.00 48.51 | AAAA |
| | 2671 | CZ | PHE | 335 | 22.373 | 48.309 | 49.296 | 1.00 40.44 | AAAA |
| MOTA | | | PHE | 335 | 24.033 | 51.000 | 45.839 | 1.00 54.52 | AAAA |
| MOTA | 2672 | C | | 335 | 23.603 | 49.939 | 45.379 | 1.00 59.24 | AAAA |
| MOTA | 2673 | 0 | PHE | | 23.302 | 52.108 | 45.888 | 1.00 50.94 | AAAA |
| ATOM | 2674 | N | GLU | 336 | | 52.119 | 45.406 | 1.00 57.05 | AAAA |
| ATOM | 2675 | CA | GLU | 336 | 21.923 | | 43.924 | 1.00 60.27 | AAAA |
| ATOM | 2676 | CB | GLU | 336 | 21.853 | 51.751 | 43.422 | 1.00 68.55 | AAAA |
| MOTA | 2677 | CG | GLU | 336 | 20.430 | 51:627 | | 1.00 80.03 | AAAA |
| ATOM | 2678 | CD | GLU | 336 | 20.352 | 51.126 | 42.001 | | |
| ATOM | 2679 | OE1 | GLU | 336 | 20.860 | 50.013 | 41.735 | 1.00 84.64 | AAAA |
| ATÓM | 2680 | | GLU | 336 | 19.777 | 51.841 | 41.153 | 1.00 80.68 | AAAA |
| | 2681 | c | GLU | 336 | 21.065 | 51.135 | 46.201 | 1.00 55.73 | AAAA |
| ATOM | 2682 | ŏ | GLU | 336 | 21.219 | 49.917. | 46.089 | 1.00 51.33 | AAAA |
| ATOM | | N | GLU | 337 | 20.151 | 51.679 | 46.992 | 1.00 49.54 | AAAA |
| MOTA | 2683 | | | 337 | 19.267 | 50.880 | 47.821 | 1.00 48.19 | AAAA |
| MOTA | 2684 | CA | GLU | | 18.510 | 51.822 | 48.764 | 1.00 47.73 | AAAA |
| MOTA | 2685 | CB | GLU | 337 | | 51.205 | 50.077 | 1.00 55.69 | AAAA |
| MOTA | 2686 | CG | GLU | 337 | 18.084 | 50.720 | 50.904 | 1.00 50.17 | AAAA |
| MOTA | 2687 | CD | GLU | . 337 | 19.269 | | 51.345 | 1.00 36.03 | AAAA |
| ATOM | 2688 | | GLU | 337 | 20.111 | 51.548 | | 1.00 51.25 | AAAA |
| ATOM | 2689 | OE2 | GLU | 337 | 19.358 | 49.494 | 51.105 | | AAAA |
| ATOM | 2690 | С | GLU | 337 | 18.294 | 50.083 | 46.936 | 1.00 49.13 | |
| MOTA | 2691 | 0 | GLU | 337 | 17.816 | 50.588 | 45.916 | 1.00 48.61 | AAAA |
| | 2692 | N | PHE | 338 | 18.015 | 48.837 | 47.313 | 1.00 48.15 | AAAA |
| MOTA | | | | 338 | 17.092 | 48.000 | 46.547 | 1.00 48.12 | AAAA |
| MOTA | 2693 | CA | PHE | 338 | 16.870 | 46.658 | 47.249 | 1.00 - 54.54 | AAAA |
| MOTA | 2694 | CB | PHE | | 15.883 | 45.777 | 46.548 | 1.00 57.22 | AAAA |
| ATOM | 2695 | CG | PHE | 338 | | 45.366 | 45.243 | 1.00 60.01 | AAAA |
| ATOM: | 2696 | | PHE | 338 | 16.115 | | | 1.00 55.04 | AAAA |
| MOTA | 2697 | | PHE | 338 | 14.699 | 45.398 | 47.171 | 1.00 60.84 | AAAA |
| ATOM | 2698 | CE1 | PHE | 338 | 15.185 | 44.597 | 44.566 | 1.00 00.04 | AAAA |
| ATOM | 2699 | | PHE | 338 | 13.758 | 44.624 | 46.497 | 1.00 59.41 | |
| | 2700 | CZ | PHE | 338 | 14.002 | 44.224 | 45.189 | 1.00 57.18 | AAAA |
| MOTA | | c | PHE | 338 | 15.755 | 48.714 | | 1.00 45.46 | AAAA |
| MOTA | 2701 | | | 338 | 15.274 | 48.900 | | 1.00 51.11 | AAAA |
| ATOM | 2702 | 0 | PHE | 339 | 15.154 | 49.098 | | 1.00 40.38 | AAAA |
| MOTA | 2703 | N | ASP | | 13.890 | 49 820 | 47.488 | 1.00 49.97 | AAAA |
| ATOM. | 2704 | CA | ASP | 339 | | | | 1.00 53.23 | AAAA |
| MOTA | 2705 | CB | ASP | | 13.270 | 49.821 | 40.000 | 1.00 57.40 | AAAA |
| ATOM | 2706 | CG | ASP | 339 | 12.000 | 50.659 | 48.968 | 1.00 57710 | •• |
| | | - | | - | | | | | |

| ATOM | 2707 | | 11 2 CD | 220 | | | | | |
|--------------|--------------|-----|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| | 2708 | | Ol ASP | | 12.039 | | | | AAAA |
| ATOM | | | 2 ASP | | 10.963 | | | 1.00 51.15 | AAAA |
| ATOM | 2709 | | ASP | | 14.215 | | 47.076 | 1.00 55.06 | AAAA |
| ATOM | 2710 | | ASP | 339 | 14.994 | | 47.748 | 1.00 56.47 | AAAA |
| ATOM | 2711 | | ASP | 340 | 13.623 | | 45.978 | 1.00 58.46 | AAAA |
| MOTA | 2712 | | | 340 | 13.874 | | | | AAAA |
| Mota | 2713 | | | 340 | 12.683 | | 44.664 | | AAAA |
| ATOM | 2714 | _ | ASP | 340 | 12.611 | | 43.295 | | AAAA |
| ATOM | 2715 | OL | 1 ASP | 340 | 12.528 | 51.667 | | | AAAA |
| MOTA | 2716 | OD | 2 ASP | 340 | 12.640 | 53.655 | | | AAAA |
| MOTA | 2717 | С | ASP | 340 | 14.209 | 54.072 | | | AAAA |
| MOTA | 2718 | 0 | ASP | 340 | 15.204 | | | 1.00 70.13 | |
| ATOM | 2719 | N | GLU | 341 | 13.392 | | | | AAAA |
| ATOM | 2720 | CA | GLU | 341 | 13.668 | | | 1.00 67.87 | AAAA |
| MOTA | 2721 | CB | GLU | 341 | 13.195 | | 48.278 | | AAAA |
| ATOM | 2722 | CG | | 341 | 13.502 | | 49.298 | 1.00 82.72 | AAAA |
| ATOM | 2723 | CD | | 341 | 13.162 | | 48.790 | 1.00 90.80 | AAAA |
| ATOM | 2724 | OE | 1 GLU | 341 | 11.988 | | 48.431 | 1.00 90.38 | AAAA |
| MOTA | 2725 | | 2 GLU | 341 | 14.072 | 59.835 | 48.752 | 1.00 93.36 | AAAA |
| MOTA | 2726 | С | GLU | 341 | 13.101 | 54.719 | 50.058 | 1.00 60.22 | AAAA |
| ATOM | 2727 | Ō | GLU | 341 | 11.929 | 54.955 | 50.347 | | AAAA |
| ATOM | 2728 | N | VAL | 342 | 13.956 | 54.144 | 50.897 | 1.00 58.81 | AAAA |
| ATOM | 2729 | CA | VAL | 342 | 13.594 | 53.781 | 52.262 | 1.00 57.28 | AAAA |
| ATOM | 2730 | CB | VAL | 342 | 14.195 | 52.419 | 52.669 | 1.00 52.09 | AAAA |
| MOTA | 2731 | | l VAL | 342 | 13.730 | 52.042 | | 1.00 53.17 | AAAA |
| ATOM | 2732 | | VAL | 342 | 13.815 | 51.356 | 54.070 | 1.00 46.16 | AAAA |
| ATOM | 2733 | C | VAL | 342 | 14.263 | 54.843 | 51.663 53.124 | 1.00 59.09 | AAAA |
| ATOM | 2734 | Ō | VAL | 342 | 13.763 | 55.230 | 54.185 | 1.00 53.31 1.00 57.79 | AAAA |
| ATOM | 2735 | N | ASP | 343 | 15.398 | 55.306 | 52.610 | 1.00 46.24 | AAAA |
| MOTA | 2736 | CA | ASP | 343 | 16.268 | 56.289 | 53.243 | 1.00 42.60 | AAAA AAAA |
| MOTA | 2737 | CB | ASP | 343 | 15.521 | 57.510 | 53.781 | 1.00 43.88 | AAAA |
| MOTA | 2738 | CG | ASP | 343 | 16.480 | 58.581 | 54.290 | 1.00 46.82 | AAAA |
| MOTA | 2739 | ODI | ASP | 343 | 16.028 | 59.581 | 54.887 | 1.00 46.16 | AAAA |
| MOTA | 2740 | OD2 | ASP | 343 . | | 58.414 | 54.075 | 1.00 33.01 | AAAA |
| ATOM | . 2741 | С | ASP | 343 | 17.012 | 55.636 | 54.395 | 1.00 35.45 | AAAA |
| MOTA | 2742 | 0 | ASP | 343 | 16.487 | 55.480 | 55.502 | 1.00 29.39 | AAAA |
| MOTA | 2743 | N | ARG | 344 | 18.247 | 55.249 | 54.124 | 1.00 30.51 | AAAA |
| ATOM | 2744 | CA | ARG | 344 | 19.059 | 54.613 | 55.140 | 1.00 29.43 | AAAA |
| ATOM | 2745 | CB | ARG | 344 | 19.736 | 53.377 | 54.561 | 1.00 30.10 | AAAA |
| ATOM | 2746 | CG | ARG | 344 | 18.803 | 52.258 | 54.180 | 1.00 33.95 | AAAA |
| ATOM | 2747 2748 | CD | ARG | 344 | 17.981 | 51.770 | 55.365 | 1.00 20.92 | AAAA |
| ATOM ATOM | 2748 | NE | ARG | 344 | 17.120 | 50.673 | 54.936 | 1.00 29.72 | AAAA |
| ATOM | 2750 | CZ | ARG | 344 | 16.110 | 50.176 | 55.639 | 1.00 29.13 | AAAA |
| MOTA | 2751 | NH2 | ARG | 344 | 15.805 | 50.668 | 56.835 | 1.00 29.63 | AAAA |
| ATOM | 2752 | C | ARG ARG | 344 | 15.379 | 49.198 | 55.120 | 1.00 27.19 | AAAA: |
| ATOM | 2753 | ō | ARG | 344 344 | 20.116 | 55.769 | 55.660 | 1.00 34.31 | AAAA |
| ATOM | 2754 | N | SER | 345 | 21.005 20.011 | 5557 | 56.391 | 1.00 29.09 | AAAA |
| MOTA | 2755 | CA | SER | 345 | 20.999 | 56. 45 | 55.294 | 1.00 28.34 | AAAA |
| ATOM | 2756 | СВ | SER | 345 | 20.669 | 57.839 59.199 | 55.715 | 1.00 30.95 | AAAA |
| ATOM | 2757 | OG | SER | 345 | 19.429 | 59.648 | 55.109 55.610 | 1.00 29.56 | AAAA |
| ATOM | 2758 | c | SER | 345 | 21.137 | 57.988 | 57.230 | | AAAA |
| ATOM | 2759 | ō | SER | 345 | 22.155 | 58.488 | 57.718 | 1.00 30.92 | AAAA |
| MOTA | 2760 | N | TYR | 346 | 20.116 | 57.576 | 57.975 | 1.00 31.15 | AAAA |
| ATOM | 2761 | CA | TYR | 346 | 20.158 | 57.659 | 59.433 | 1.00 25.64 1.00 26.81 | . AAAA |
| MOTA | 2762 | СВ | TYR | 346 | 18.823 | 57.189 | 60.006 | 1.00 26.81 | AAAA |
| ATOM | 2763 | CG | TYR | 346 | 18.529 | 55.723 | 59.716 | 1.00 27.35 | AAAA |
| ATOM | 2764 | CD1 | | 346 | 19.003 | 54.708 | 60.556 | 1.00 24.87 | AAAA |
| MOTA | 2765 | CE1 | | 346 | 18.744 | 53.352 | 60.278 | 1.00 24.87 | AAAA AAAA |
| ATOM | 2766 | CD2 | | 346 | 17.795 | 55.358 | 58.588 | 1.00 27.70 | AAAA |
| ATOM | 2767 | CE2 | | 346 | 17.533 | 54.008 | 58.297 | 1.00 27.70 | AAAA |
| ATOM | 2768 | cz | TYR | 346 | 18.008 | 53.015 | 59.145 | 1.00 23.75 | AAAA |
| ATOM | 2769 | ОН | TYR | 346 | 17.737 | 51.691 | 58.855 | 1.00 26.06 | AAAA |
| ATOM . | 2770 | C | TYR | 346 | 21.277 | 56.766 | 59.977 | 1.00 25.57 | AAAA |
| ATOM | 2771 | | TYR | 346 | 21.769 | 56.970 | 61.085 | 1.00 28.07 | AAAA |
| ATOM | 2772 | N | MET . | 347 | 21.666 | 55.761 | 59.198 | 1.00 29.08 | AAAA |
| ~ | | | | • | | | - | - | |

| | | | | 2.42 | 22.720 | 54.837 | 59.622 | 1.00 24.19 | AAAA |
|-------------------|--------------|-----------|--------------|------------|------------------|------------------|------------------|---|--------------|
| MOTA | 2773 | | MET | 347 | 22.720 | 53.678 | 58.628 | 1.00 24.87 | AAAA |
| MOTA | 2774 | | MET | 347 | 21.609 | 52.806 | 58.543 | 1.00 23.66 | AAAA |
| ATOM | 2775 | | MET | 347 | 21.780 | 51.503 | 57.267 | 1.00 27.02 | AAAA |
| MOTA | 2776 | | MET | 347 | 22.115 | 52.375 | 55.896 | 1.00 37.69 | AAAA |
| MOTA | 2777 | | MET | 347 | 24.054 | 55.540 | 59.737 | 1.00 29.45 | AAAA |
| MOTA | 2778 | | MET | 347 | 24.937 | 55.092 | 60.479 | 1.00 28.08 | AAAA |
| ATOM | 2779 | | MET | 347 | 24.188 | 56.650 | 59.007 | 1.00 23.71 | AAAA |
| ATOM | 2780 | N | LEU | 348 348 | 25.418 | 57.446 | 58.998 | 1.00 34.11 | AAAA |
| MOTA | 2781 | CA | LEU | 348 | 25.463 | 58.351 | 57.757 | 1.00 25.37 | AAAA |
| MOTA | 2782 | CB | LEU | 348 | 25.320 | 57.785 | 56.344 | 1.00 30.38 | AAAA |
| MOTA | 2783 | CG CD1 | LEU | 348 | 25.307 | 58.944 | 55.340 | 1.00 27.44 | AAAA |
| MOTA | 2784 | CD2 | | 348 | 26.459 | 56.814 | 56.041 | 1.00 36.44 | AAAA |
| MOTA | 2785 | CDZ | LEU | 348 | 25.507 | 58.332 | 60.237 | 1.00 36.09 | AAAA |
| ATOM | 2786 | 0 | LEU | 348 | 26.561 | 58.894 | 60.539 | 1.00 33.30 | AAAA AAAA |
| ATOM | 2787 2788 | N | GLU | 349 | 24.394 | 58.445 | 60.953 | 1.00 30.51 | AAAA |
| ATOM | 2789 | CA | GLU | 349 | 24.313 | 59.292 | 62.136 | 1.00 35.53 | AAAA . |
| MOTA | 2790 | CB | GLU | 349 | 22.908 | 59.896 | 62.217 | 1.00 31.35 1.00 29.09 | AAAA |
| MOTA | 2791 | CG | GLU | 349 | 22.518 | 60.717 | 61.006 | 1.00 29.09 | AAAA |
| MOTA MOTA | 2792 | CD | GLU | 349 | 23.481 | 61.859 | 60.746 | 1.00 31.78 | AAAA |
| ATOM | 2793 | | GLU | 349 | 23.937 | 62.476 | 61.730 | 1.00 30.67 | AAAA |
| ATOM | 2794 | OE2 | GLU | 349 | 23.766 | 62.155 | 59.569 | 1.00 38.48 | AAAA |
| MOTA | 2795 | С | GLU | 349 | 24.663 | 58.633 | 63.471 64.502 | 1.00 40.12 | AAAA |
| MOTA | 2796 | 0 | GLU | 349 | 24.727 | 59.303 | 63.461 | 1.00 33.58 | AAAA |
| ATOM | 2797 | N | THR | 350 | 24.878 | 57.326 | 64.681 | 1.00 29.74 | AAAA |
| ATOM | 2798 | CA | THR | 350 | 25.221 | 56.612 56.363 | 65.559 | 1.00 35.91 | AAAA |
| MOTA | 2799 | CB | THR | 350 | 23.992 | 57.615 | 65.952 | 1.00 45.03 | AAAA |
| MOTA | 2800 | | THR | 350 | 23.421 24.382 | 55.586 | 66.806 | 1.00 49.48 | AAAA |
| MOTA | 2801 | | THR | 350 | 25.821 | 55.267 | 64.330 | 1.00 30.63 | AAAA |
| MOTA | 2802 | C | THR | 350 | 25.535 | 54.709 | 63.274 | 1.00 26.62 | AAAA |
| MOTA | 2803 | 0 | THR | 350 | 26.644 | 54.740 | 65.225 | 1.00 29.07 | AAAA |
| MOTA | 2804 | N | LEU | 351 351 | 27.271 | 53.461 | 64.972 | 1.00 24.59 | AAAA |
| MOTA | 2805 | CA | LEU | 351 | 28.584 | 53.367 | 65.757 | 1.00 29.91 | AAAA |
| MOTA | 2806 | CB CG | LEU | 351 | 29.591 | 52.327 | 65.267 | 1.00 39.62 | AAAA |
| MOTA | 2807 | | LEU | 351 | 30.887 | 52.467 | 66.039 | 1.00 37.09 | AAAA AAAA |
| MOTA | 2808 2809 | | LEU | 351 | 29.024 | 50.935 | 65.415 | 1.00 54.03 | AAAA |
| MOTA | 2810 | C | LEU | 351 | 26.314 | 52.336 | 65.377 | 1.00 29.71 1.00 30.53 | AAAA |
| MOTA | 2811 | ō | LEU | 351 | 26.130 | 51.364 | 64.641 | 1.00 28.64 | AAAA |
| MOTA MOTA | 2812 | N | LYS | 352 | 25.697 | 52.481 | 66.543 | 1.00 28.04 | AAAA |
| ATOM | 2813 | CA | LYS | 352 | 24.763 | 51.479 | 67.061 68.581 | 1.00 27.37 | AAAA |
| ATOM | 2814 | CB | LYS | 352 | 24.913 | 51.381 | 69.034 | 1.00 43.48 | AAAA |
| ATOM | 2815 | CG | LYS | 352 | 26.230 | 50.787 51.068 | | 1.00 46.77 | AAAA |
| ATOM | 2816 | CD | LYS | 352 | 26.536 | | | | AAAA |
| ATOM | 2817 | CE | LYS | 352 | 25.484 | | | 1.00 62.08 | AAAA |
| A OM | 2818 | NZ | LYS | 352 | 25.850 23.330 | | | 1.00 32.49 | AAAA |
| A L'OM | 2819 | C | LYS | 352 | 22.953 | | | 1.00 31.90 | AAAA |
| A ₁ OM | 2820 | 0 | LYS | 352 | 22.525 | | | 1.00 31.44 | AAAA |
| ATOM | 2821 | N | ASP | 353 353 | 21.136 | | | 1.00 26.50 | AAAA |
| MOTA | 2822 | CA | ASP ASP | 353 | 20.543 | | | 1.00 50.09 | AAAA |
| MOTA | 2823 | CB | ASP | 353 | 20.880 | | | . 1.00 52.79 | AAAA |
| MOTA | 2824 | CG | ASP 1 ASP | 353 | 21.980 | | 64.109 | 1.00 58.55 | AAAA |
| MOTA | 2825 | OD. | 2 ASP | 353 | 20.040 | | 64.984 | 1.00 73.19 | AAAA AAAA |
| ATOM | 2826 | | ASP | 353 | 20.328 | | 67.257 | | AAAA |
| MOTA | 2827 | C O | ASP | 353 | 20.806 | | | | AAAA |
| MOTA | 2828 2829 | | PRO | 354 | 19.118 | 51.481 | | | AAAA |
| MOTA | 2830 | | | 354 | 18.428 | 52.429 | | | AAAA |
| MOTA | 2831 | | | 354 | 18.276 | 51.190 | 68.547 | | AAAA |
| MOTA | 2832 | | | 354 | 17.09 | | | | AAAA |
| MOTA | 2833 | | | 354 | 16.974 | | | | AAAA |
| MOTA MOTA | 2834 | _ | PRO | 354 | 17.838 | | | | AAAA |
| ATOM | 2835 | _ | PRO | 354 | 17.829 | | | | AAAA |
| ATOM | | | TRP | 355 | 17.48 | 49.19 | | | AAAA |
| ATOM | | _ | | 355. | 17.010 | | | | AAAA |
| ATOM | | | TRP | 355 | 16.65 | 3 47.36 | , , 1.0,, | • • • • • • • · · · · · · · · · · · · · | • |
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| ATOM 2839 CG TRP 355 17.844 46.946 71.832 1.00 49.97 AAAA ATOM 2840 CD2 TRP 355 18.364 45.622 71.905 1.00 46.66 AAAA ATOM 2841 CEZ TRP 355 19.567 45.682 72.639 1.00 54.73 AAAA ATOM 2842 CE3 TRP 355 19.567 45.682 72.639 1.00 54.73 AAAA ATOM 2842 CE3 TRP 355 19.567 45.682 72.639 1.00 55.10 AAAA ATOM 2843 CD1 TRP 355 18.723 47.746 72.507 1.00 56.10 AAAA ATOM 2844 NEI TRP 355 19.565 46.991 72.997 1.00 56.07 AAAA ATOM 2845 CZ2 TRP 355 19.568 46.991 72.997 1.00 55.25 AAAA ATOM 2846 CZ3 TRP 355 19.868 41.556 72.405 1.00 50.525 AAAA ATOM 2846 CZ3 TRP 355 19.868 41.556 72.405 1.00 50.525 AAAA ATOM 2848 CZ TRP 355 19.868 41.556 72.405 1.00 50.524 AAAA ATOM 2848 CZ TRP 355 19.868 41.556 72.405 1.00 50.524 AAAA ATOM 2848 CZ TRP 355 19.868 41.556 67.2405 1.00 50.68 AAAA ATOM 2848 CZ TRP 355 19.868 41.556 67.2405 1.00 20.312 AAAA ATOM 2851 CA ARG 356 15.947 46.508 68.550 1.00 20.312 AAAA ATOM 2852 CB ARG 356 14.892 46.996 65.935 1.00 20.306 AAAA ATOM 2852 CB ARG 356 14.892 46.996 65.935 1.00 20.306 AAAA ATOM 2855 CG ARG 356 16.291 47.212 64.108 1.00 22.96 AAAA ATOM 2855 CC ARG 356 16.291 47.212 64.108 1.00 22.97 AAAA ATOM 2855 NP ARG 356 16.291 47.212 64.108 1.00 22.97 AAAA ATOM 2855 NP ARG 356 16.291 47.212 64.108 1.00 22.95 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 18.153 49.891 62.418 1.00 22.95 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.57 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.59 AAAA ATOM 2859 CC ARG 356 17.733 48.668 62.724 1.00 22.59 AAAA ATOM 2850 CC ARG 356 17.733 48.668 62.724 1.00 22.59 AAAA ATOM 2850 CC ARG 356 17.733 48.668 62.724 1.00 22.59 AAAA ATOM 2850 CC ARG 356 17.733 48.668 62.724 1.00 22.59 AA | ATOM | 2839 | 00 | , m | | | | | | | | | |
|--|------|------|-----|-----|-----|---|-------|--------|--------|------|-------|---|--------|
| ATOM 2841 CE2 TRP 355 19.567 45.682 72.639 1.00 54.73 AAAAA ATOM 2842 CE3 TRP 355 17.931 44.386 71.419 1.00 54.13 AAAAA ATOM 2843 CD1 TRP 355 18.723 47.746 72.507 1.00 55.10 AAAAA ATOM 2844 NE1 TRP 355 18.723 47.746 72.507 1.00 55.07 AAAAA ATOM 2846 CE3 TRP 355 19.765 46.991 72.507 1.00 55.07 AAAAA ATOM 2846 CE3 TRP 355 19.765 44.356 72.897 1.00 55.07 AAAAA ATOM 2846 CE3 TRP 355 19.765 44.356 72.897 1.00 55.07 AAAAA ATOM 2847 CL2 TRP 355 19.887 43.356 72.405 1.00 50.64 AAAAA ATOM 2848 C TRP 355 15.789 47.712 68.756 1.00 50.54 AAAAA ATOM 2848 C TRP 355 15.789 47.712 68.500 1.00 20.312 AAAAA ATOM 2851 CA ARG 356 15.547 46.508 68.550 1.00 29.41 AAAAA ATOM 2851 CA ARG 356 14.892 46.096 65.935 1.00 23.90 AAAAA ATOM 2852 CB ARG 356 14.892 46.096 65.935 1.00 23.90 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 63.935 1.00 29.64 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 63.935 1.00 29.66 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 62.395 1.00 29.92 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 62.395 1.00 29.92 AAAAA ATOM 2856 CZ ARG 356 16.291 47.212 64.096 62.006 1.00 22.15 AAAAA ATOM 2857 NH1 ARG 356 18.209 47.616 62.066 1.00 24.73 AAAA ATOM 2856 CZ ARG 356 18.153 48.693 63.686 1.00 24.73 AAAA ATOM 2856 CZ ARG 356 18.153 48.993 69.085 1.00 23.91 AAAAA ATOM 2856 CZ ARG 356 18.153 48.993 69.085 1.00 23.91 AAAAA ATOM 2856 CZ ARG 356 18.153 48.993 69.085 1.00 23.91 AAAAA ATOM 2856 CZ ARG 356 18.153 48.993 69.085 1.00 23.91 AAAAA ATOM 2856 CZ ARG 356 13.785 49.891 62.418 1.00 22.15 AAAAA ATOM 2866 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2866 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2866 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2866 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2866 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2866 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2868 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2868 CZ ARG 356 13.785 44.993 69.085 1.00 23.91 AAAAA ATOM 2886 CZ ARG 356 13.785 34.993 69.085 1.00 23.91 AAAAA | | | | | | | | | | | | | AAAA |
| ATOM 2842 CE3 TRP 355 17.931 44.386 71.419 1.00 36.90 AAAAA ATOM 2843 CD1 TRP 355 18.723 47.766 72.507 1.00 56.10 AAAAA ATOM 2844 NEI TRP 355 19.765 46.991 72.997 1.00 56.07 AAAA ATOM 2846 CZ3 TRP 355 19.765 46.991 72.997 1.00 56.07 AAAA ATOM 2846 CZ3 TRP 355 19.765 46.991 72.997 1.00 55.25 AAAAA ATOM 2846 CZ3 TRP 355 19.887 34.356 71.674 1.00 55.25 AAAAA ATOM 2848 C TRP 355 15.789 47.712 68.776 1.00 50.74 AAAA ATOM 2848 C TRP 355 15.789 47.712 68.776 1.00 50.68 AAAAA ATOM 2848 C TRP 355 15.5096 48.705 68.550 1.00 29.41 AAAAA ATOM 2851 CA ARG 356 14.413 46.291 67.387 1.00 23.90 AAAAA ATOM 2851 CA ARG 356 14.413 46.291 67.387 1.00 23.90 AAAAA ATOM 2852 CD ARG 356 14.413 66.291 77.385 65.393 1.00 23.90 AAAAA ATOM 2853 CO ARG 356 15.505 47.385 65.393 1.00 22.66 AAAAA ATOM 2855 CD ARG 356 16.833 48.503 66.886 1.00 22.156 AAAAA ATOM 2855 NE ARG 356 16.833 48.503 66.886 1.00 22.157 AAAAA ATOM 2855 NE ARG 356 16.833 48.503 66.886 1.00 24.73 AAAAA ATOM 2855 NE ARG 356 16.833 48.503 66.886 1.00 24.73 AAAAA ATOM 2855 NE ARG 356 18.209 47.616 62.066 1.00 22.157 AAAAA ATOM 2858 NHIZ ARG 356 18.209 47.616 62.066 1.00 22.157 AAAAA ATOM 2858 NHIZ ARG 356 18.209 47.616 62.066 1.00 22.157 AAAAA ATOM 2858 NHIZ ARG 356 18.209 47.616 62.066 1.00 22.157 AAAAA ATOM 2866 C A GLV 357 12.211 44.994 67.878 1.00 22.89 AAAAA ATOM 2866 C A GLV 357 11.388 49.891 62.00 6 | | | | | | | | | | | | | |
| ATOM 2843 CD1 TRP 355 18.723 47.746 72.507 1.00 35.10 AAAA ATOM 2844 NEI TRP 355 19.765 46.991 72.507 1.00 55.07 AAAA ATOM 2846 C23 TRP 355 20.340 44.552 72.897 1.00 55.07 AAAA ATOM 2846 C23 TRP 355 18.696 43.267 71.674 1.00 55.05 AAAA ATOM 2847 CH2 TRP 355 19.887 43.356 72.405 1.00 50.54 AAAA ATOM 2848 C TRP 355 19.887 43.356 72.405 1.00 50.68 AAAA ATOM 2848 C TRP 355 15.789 47.712 68.776 1.00 20.312 AAAA ATOM 2849 O TRP 355 15.789 47.712 68.625 1.00 29.41 AAAA ATOM 2850 N ARG 356 15.547 46.508 68.500 1.00 29.41 AAAA ATOM 2851 CA ARG 356 14.892 46.096 65.935 1.00 23.91 AAAA ATOM 2852 CB ARG 356 14.892 46.096 65.935 1.00 22.66 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 65.935 1.00 22.66 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 62.351 1.00 22.06 AAAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 10.00 22.55 AAAA ATOM 2855 NE ARG 356 16.291 47.212 64.096 10.00 22.55 AAAA ATOM 2855 NE ARG 356 18.209 47.616 62.066 1.00 22.15 AAAAA ATOM 2855 NE ARG 356 18.209 47.616 62.066 1.00 22.15 AAAAA ATOM 2856 CZ ARG 356 18.153 48.991 62.418 1.00 22.59 AAAAA ATOM 2856 NPL ARG 356 18.153 49.891 62.418 1.00 22.59 AAAAA ATOM 2856 NPL ARG 356 18.153 49.891 62.418 1.00 22.59 AAAAA ATOM 2856 NPL ARG 356 13.781 44.994 67.878 1.00 22.357 AAAAA ATOM 2856 NPL ARG 356 13.781 44.994 67.878 1.00 22.25 AAAAA ATOM 2866 C C ARG 356 13.785 14.995 67.189 1.00 22.25 AAAAA ATOM 2866 C C ARG 356 13.785 14.995 67.788 1.00 22.25 AAAAA ATOM 2866 O ARG 356 13.785 14.995 67.788 1.00 22.25 AAAAA ATOM 2866 C C GLY 357 11.388 10.544 42.797 70.265 1.00 23.91 AAAAA ATOM 2866 C C GLY 357 11.388 10.544 42.797 70.265 1.00 23.91 AAAAA ATOM 2866 C C GLY 357 11.388 10.544 42.797 70.265 1.00 23.91 AAAAA ATOM 2866 C C GLY 358 8.800 41.274 70.920 1.00 30.03 AAAAA ATOM 2866 C C GLY 358 8.800 41.274 70.920 1.00 30.03 AAAAA ATOM 2867 C GLY 357 89.91 89.918 42.917 70.265 1.00 22.22 AAAAA ATOM 2868 C C GLY 357 89.918 89.918 42.919 70.010 30.03 AAAAA ATOM 2868 C C GLY 357 89.918 89.918 42.919 70.01 30.920 30.93 AAAAA ATOM 2889 C C GLY 357 89.918 89.918 42.919 70. | | | | | | | | | | _ | | | |
| ARTON 2844 NEI TRP 355 19.765 46.991 72.997 1.00 56.07 AAAA ARTON 2845 C22 TRP 355 19.867 46.991 72.997 1.00 56.07 AAAA ARTON 2846 C23 TRP 355 18.696 43.267 71.674 1.00 50.74 AAAA ARTON 2847 CH2 TRP 355 19.887 43.355 71.674 1.00 50.74 AAAA ARTON 2848 C TRP 355 15.789 47.712 68.776 1.00 50.68 AAAAA ARTON 2849 0 TRP 355 15.5096 48.705 68.706 1.00 50.68 AAAAA ARTON 2850 N ARG 356 15.547 46.508 68.550 1.00 29.41 AAAA ARTON 2851 CA ARG 356 15.547 46.508 68.253 1.00 29.41 AAAA ARTON 2851 CA ARG 356 14.413 46.237 67.387 1.00 23.90 AAAA ARTON 2852 CD ARG 356 14.413 66.237 67.387 1.00 23.90 AAAA ARTON 2852 CD ARG 356 16.291 47.212 66.956 65.935 1.00 23.90 AAAA ARTON 2855 NE ARG 356 16.291 47.212 66.906 65.935 1.00 23.90 AAAAA ARTON 2855 NE ARG 356 16.291 47.212 66.006 10.00 23.90 AAAAA ARTON 2855 NE ARG 356 16.833 48.503 62.666 1.00 24.73 AAAAA ARTON 2855 NE ARG 356 16.833 48.503 62.666 1.00 24.73 AAAAA ARTON 2855 NE ARG 356 16.833 48.503 62.666 1.00 24.73 AAAAA ARTON 2855 NE ARG 356 17.733 48.668 62.666 1.00 24.73 AAAAA ARTON 2859 C ARG 356 18.159 49.891 62.488 1.00 22.155 AAAAA ARTON 2858 NEL ARG 356 13.781 49.891 62.488 1.00 22.155 AAAAA ARTON 2858 NEL ARG 356 13.781 49.891 62.488 1.00 22.155 AAAAA ARTON 2858 NEL ARG 356 13.781 49.891 62.488 1.00 22.155 AAAAA ARTON 2860 O ARG 356 13.781 44.994 67.898 10.00 22.155 AAAAA ARTON 2860 O ARG 356 13.785 43.995 69.655 1.00 22.157 AAAAA ARTON 2866 CA GLV 357 11.388 43.671 62.488 1.00 22.22 AAAAA ARTON 2866 O ARG 356 13.781 44.994 67.898 10.00 24.89 AAAAA ARTON 2866 CA GLV 357 11.388 14.994 67.898 10.00 24.89 AAAAA ARTON 2866 CA GLV 357 11.388 19.504 64.2997 70.265 10.00 26.90 AAAAA ARTON 2866 CA GLV 357 11.388 19.544 67.900 67.15 10.00 26.70 AAAAA ARTON 2866 CA GLV 357 11.388 19.544 67.900 67.15 10.00 26.70 AAAAA ARTON 2866 CA GLV 358 10.544 42.997 70.265 10.00 26.70 AAAAA ARTON 2867 C GLU 3599 7.601 40.747 70.715 1.00 26.71 AAAAA ARTON 2870 C GLU 3599 7.601 40.747 70.701 1.00 20.00 20.00 AAAAA ARTON 2870 C GLU 3599 7.601 40.747 70.701 1.00 20.00 20.00 AAAAA ARTON 2888 C G GL | | | | | | | | | | | | | AAAA |
| ARTON 2846 C23 TRP 355 20.340 44.552 72.897 1.00 55.25 AAAA ARTON 2846 C23 TRP 355 18.696 43.267 71.674 1.00 55.25 AAAA ARTON 2848 C TRP 355 19.887 43.356 72.405 1.00 50.68 AAAA ARTON 2848 C TRP 355 15.789 47.712 68.550 1.00 21.21 AAAA ARTON 2849 O TRP 355 15.789 47.712 68.550 1.00 23.90 AAAA ARTON 2850 N ARG 356 15.547 46.508 68.550 1.00 23.90 AAAAA ARTON 2851 CA ARG 356 15.547 46.508 68.550 1.00 23.90 AAAAA ARTON 2851 CA ARG 356 16.831 46.237 67.387 1.00 23.90 AAAAA ARTON 2853 CG ARG 356 16.831 46.237 67.387 1.00 22.66 AAAAA ARTON 2855 NE ARG 356 16.831 46.508 65.935 1.00 22.66 AAAAA ARTON 2855 NE ARG 356 16.831 48.503 61.686 1.00 28.92 AAAAA ARTON 2855 NE ARG 356 16.831 48.503 61.686 1.00 22.57 AAAAA ARTON 2855 NE ARG 356 16.831 48.503 61.686 1.00 22.57 AAAAA ARTON 2857 NHI ARG 356 18.209 47.616 62.066 1.00 22.15 AAAA ARTON 2858 NE ARG 356 18.159 49.891 62.418 1.00 22.59 AAAAA ARTON 2859 C ARG 356 13.781 44.944 67.878 1.00 22.55 AAAAA ARTON 2850 C ARG 356 13.781 44.944 67.878 1.00 22.55 AAAAA ARTON 2850 NA GA 356 13.785 43.925 67.189 1.00 22.25 AAAAA ARTON 2850 C ARG 356 13.781 44.993 69.085 1.00 22.25 AAAAA ARTON 2861 N GLY 357 11.231 44.993 69.085 1.00 22.95 AAAAA ARTON 2861 N GLY 357 11.231 44.993 69.085 1.00 22.95 AAAAA ARTON 2865 N GLY 357 11.383 43.671 69.085 1.00 29.87 AAAAA ARTON 2865 N GLY 358 91.18 42.551 70.188 1.00 29.87 AAAAA ARTON 2868 N GLY 358 91.18 42.551 70.188 1.00 29.87 AAAAA ARTON 2869 N GLY 358 91.18 42.551 70.188 1.00 29.87 AAAAA ARTON 2869 N GLY 358 91.18 42.551 70.188 1.00 29.87 AAAAA ARTON 2869 N GLY 358 91.18 42.551 70.188 1.00 29.87 AAAAA ARTON 2869 N GLY 358 91.18 42.551 70.188 1.00 29.97 AAAAA ARTON 2869 N GLY 358 91.18 42.551 70.188 1.00 29.97 AAAAA ARTON 2869 N GLY 358 91.18 42.551 70.188 1.00 29.97 AAAAA ARTON 2869 N GLY 358 91.87 ARTON 2870 N GLY 358 91.18 42.551 70.188 1.00 29.97 AAAAA ARTON 2870 N GLY 358 91.87 ARTON 2870 N GLY 358 91.37 N GLY 359 N GLY 359 N GLY 359 N G | | | | | | | | | | | | | |
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| ATOM 2848 C TRP 355 19,887 43,356 72,405 1.00 20.68 AAAA ATOM 2849 O TRP 355 15,789 47,712 68,776 1.00 33,12 AAAA ATOM 2850 N ARG 356 15,547 46,500 68,560 1.00 29,41 AAAA ATOM 2851 CA ARG 356 15,547 46,500 68,260 1.00 23,90 AAAAA ATOM 2851 CA ARG 356 14,892 46,096 65,935 1.00 22,96 AAAAA ATOM 2851 CA ARG 356 14,413 46,237 67,387 1.00 22,66 AAAAA ATOM 2853 CC ARG 356 14,892 46,096 65,935 1.00 22,66 AAAAA ATOM 2854 CD ARG 356 16,833 48,503 61,686 1.00 24,73 AAAA ATOM 2855 NE ARG 356 16,833 48,503 61,686 1.00 24,73 AAAA ATOM 2857 NH1 ARG 356 18,209 47,616 62,066 1.00 22,157 AAAA ATOM 2859 C ARG 356 18,209 47,616 62,066 1.00 22,157 AAAA ATOM 2859 C ARG 356 13,781 44,943 67,878 1.00 22,26 AAAAA ATOM 2859 C ARG 356 13,781 44,943 67,878 1.00 22,25 AAAAA ATOM 2861 N GLY 357 13,231 44,993 69,085 1.00 22,25 AAAAA ATOM 2861 N GLY 357 13,231 44,993 69,085 1.00 23,97 AAAAA ATOM 2863 C GLY 357 11,338 43,671 69,085 1.00 23,97 AAAAA ATOM 2865 N GLY 357 11,338 43,671 69,085 1.00 23,987 AAAAA ATOM 2865 N GLY 357 11,338 43,671 69,085 1.00 23,987 AAAAA ATOM 2866 N GLY 357 11,338 43,671 69,085 1.00 23,987 AAAAA ATOM 2866 N GLY 357 11,338 43,671 69,085 1.00 23,987 AAAAA ATOM 2866 N GLY 357 11,338 43,671 69,085 1.00 23,987 AAAAA ATOM 2866 N GLY 357 10,536 44,330 68,619 1.00 29,987 AAAAA ATOM 2866 N GLY 357 10,536 44,330 68,619 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 43,671 69,465 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 43,671 69,465 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 91,838 43,671 69,465 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 91,838 43,671 69,465 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 91,838 43,671 69,465 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 91,838 43,671 69,465 1.00 29,987 AAAAA ATOM 2866 N GLY 358 91,838 91,838 45,671 69,465 1.00 29,987 AAAAA ATOM 2867 C GLU 359 97,838 91,838 45,671 69,465 1.00 29,987 AAAAA ATOM 2868 N GLY 358 91,838 | | | | _ | | | | | | | | | |
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| ATOM 2875 OE2 GLU 359 7.804 38.323 70.628 1.00 27.35 AAAA ATOM 2876 C GLU 359 7.804 38.323 70.628 1.00 27.35 AAAA ATOM 2877 O GLU 359 8.138 38.415 69.449 1.00 22.94 AAAA ATOM 2878 N VAL 360 7.944 37.208 71.325 1.00 19.68 AAAA ATOM 2879 CA VAL 360 8.441 36.017 70.672 1.00 21.28 AAAA ATOM 2880 CB VAL 360 9.300 35.188 71.621 1.00 26.71 AAAA ATOM 2881 CG1 VAL 360 9.783 33.917 70.912 1.00 20.64 AAAA ATOM 2882 CG2 VAL 360 10.486 36.038 72.113 1.00 25.79 AAAA ATOM 2883 C VAL 360 7.228 35.202 70.197 1.00 25.51 AAAA ATOM 2883 C VAL 360 7.228 35.202 70.197 1.00 25.51 AAAA ATOM 2884 O VAL 360 6.442 34.700 71.01 1.00 19.75 AAAA ATOM 2885 N ARG 361 7.065 35.094 68.8 J 1.00 18.48 AAAA ATOM 2886 CA ARG 361 5.947 34.337 68.3 C 1.00 22.01 AAAA ATOM 2887 CB ARG 361 5.947 34.337 68.3 C 1.00 22.01 AAAA ATOM 2888 CG ARG 361 5.947 34.337 68.3 C 1.00 22.01 AAAA ATOM 2889 CD ARG 361 5.446 35.671 66.204 1.00 30.86 AAAA ATOM 2889 CD ARG 361 5.735 35.730 64.723 1.00 37.95 AAAA ATOM 2889 CD ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2891 CZ ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2892 NH1 ARG 361 8.861 36.006 62.186 1.00 19.02 AAAA ATOM 2894 C ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 2.145 31.200 70.168 1.00 50.86 AAAAA ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.86 AAAAA ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.87 AAAA ATOM 2900 CD LYS 362 2.145 31.200 70.168 1.00 50.87 AAAA ATOM 2901 CE LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.145 31.200 70.168 1.00 50.87 AAAA ATOM 2900 CD LYS 362 2.145 31.200 70.168 1.00 50.87 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 50.87 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 50.87 A | | | 0E1 | GLU | 359 | | 2.924 | 39.125 | 72.151 | | | | |
| ATOM 2877 O GLU 359 8.138 38.415 69.449 1.00 22.94 AAAA ATOM 2878 N VAL 360 7.944 37.208 71.325 1.00 19.68 AAAA ATOM 2879 CA VAL 360 8.441 36.017 70.672 1.00 21.28 AAAA ATOM 2880 CB VAL 360 9.300 35.188 71.621 1.00 26.71 AAAA ATOM 2881 CG1 VAL 360 9.783 33.917 70.912 1.00 20.64 AAAA ATOM 2881 CG2 VAL 360 10.486 36.038 72.113 1.00 25.79 AAAA ATOM 2882 CG2 VAL 360 7.228 35.202 70.197 1.00 25.51 AAAA ATOM 2883 C VAL 360 6.442 34.700 71.01 1.00 19.75 AAAA ATOM 2885 N ARG 361 7.065 35.094 68.87 1.00 18.48 AAAA ATOM 2885 CG ARG 361 5.947 34.337 68.3C 1.00 19.31 AAAA ATOM 2888 CG ARG 361 5.948 34.389 66.772 1.00 19.31 AAAA ATOM 2888 CG ARG 361 5.946 35.671 66.204 1.00 30.86 AAAA ATOM 2889 CD ARG 361 5.446 35.671 66.204 1.00 30.86 AAAA ATOM 2889 CD ARG 361 7.111 36.148 64.460 1.00 30.73 AAAA ATOM 2891 CZ ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2892 NH1 ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2892 NH1 ARG 361 8.861 36.006 62.186 1.00 19.02 AAAA ATOM 2899 C ARG 361 5.887 32.879 68.714 1.00 23.47 AAAA ATOM 2899 C ARG 361 5.887 32.879 68.714 1.00 23.47 AAAA ATOM 2897 CA ARG 361 5.887 32.879 68.714 1.00 23.47 AAAA ATOM 2897 CA ARG 361 5.887 32.879 68.714 1.00 23.47 AAAA ATOM 2897 CA ARG 361 5.887 32.879 68.714 1.00 22.91 AAAA ATOM 2897 CA ARG 361 5.887 32.879 68.714 1.00 22.91 AAAA ATOM 2897 CA ARG 361 5.897 32.879 68.714 1.00 22.91 AAAA ATOM 2897 CA ARG 361 6.926 32.255 68.968 1.00 21.79 AAAA ATOM 2897 CA ARG 361 6.926 32.255 68.968 1.00 21.79 AAAA ATOM 2897 CA ARG 361 5.897 32.879 68.714 1.00 22.91 AAAA ATOM 2898 CB AYS 362 2.981 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG AYS 362 2.981 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG AYS 362 2.981 30.570 69.070 1.00 57.51 AAAA ATOM 2900 CD AYS 362 2.996 30.014 68.202 1.00 10.0 10.0 10.0 10.0 10.0 10.0 | | | | GLU | | | 2.839 | 41.316 | 71.987 | 1.00 | 40.72 | | |
| ATOM 2878 N VAL 360 7.944 37.208 71.325 1.00 19.68 AAAA ATOM 2879 CA VAL 360 8.441 36.017 70.672 1.00 21.28 AAAA ATOM 2880 CB VAL 360 9.300 35.188 71.621 1.00 26.71 AAAA ATOM 2881 CG1 VAL 360 9.783 33.917 70.912 1.00 20.64 AAAA ATOM 2882 CG2 VAL 360 10.486 36.038 72.113 1.00 25.79 AAAA ATOM 2883 C VAL 360 7.228 35.202 70.197 1.00 25.51 AAAA ATOM 2883 C VAL 360 6.442 34.700 71.01 1.00 19.75 AAAA ATOM 2885 N ARG 361 7.065 35.094 68.87 1.00 18.48 AAAA ATOM 2885 CA ARG 361 7.065 35.094 68.87 1.00 18.48 AAAA ATOM 2886 CA ARG 361 5.947 34.337 68.3C 1.00 22.01 AAAAA ATOM 2887 CB ARG 361 5.948 34.389 66.772 1.00 19.31 AAAA ATOM 2889 CD ARG 361 5.446 35.671 66.204 1.00 30.86 AAAAA ATOM 2889 CD ARG 361 5.446 35.671 66.204 1.00 30.86 AAAAA ATOM 2899 CD ARG 361 7.111 36.148 64.460 1.00 30.73 AAAAA ATOM 2891 CZ ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2891 CZ ARG 361 6.851 36.006 62.186 1.00 19.02 AAAAA ATOM 2893 NH2 ARG 361 6.851 36.006 62.186 1.00 19.02 AAAAA ATOM 2893 NH2 ARG 361 8.861 36.704 63.081 1.00 23.47 AAAAA ATOM 2894 C ARG 361 5.897 32.879 68.714 1.00 26.11 AAAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.479 30.938 69.125 1.00 22.91 AAAAA ATOM 2899 CG LYS 362 2.981 30.570 69.070 1.00 22.91 AAAAA ATOM 2899 CG LYS 362 2.981 30.570 69.070 1.00 22.91 AAAAA ATOM 2899 CG LYS 362 2.981 30.570 69.070 1.00 22.99 AAAAA ATOM 2899 CG LYS 362 2.981 30.570 69.070 1.00 22.99 AAAAA ATOM 2899 CG LYS 362 2.981 30.570 69.070 1.00 50.86 AAAAA ATOM 2899 CG LYS 362 2.981 30.570 69.070 1.00 50.87 AAAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 50.87 AAAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 50.87 AAAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAAA ATOM 2900 CD LYS 362 2.2961 30.014 68.202 1.00 16.77 AAAAA ATOM 2900 CD LYS 362 2.200 32.715 70.157 1.00 50.87 AAAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAAA ATOM 2900 CD LYS 362 2.200 30.014 68.202 1.00 16.77 | | | | | | | | | 70.628 | 1.00 | 27.35 | | AAAA |
| ATOM 2887 CA VAL 360 8.441 36.017 70.672 1.00 21.28 AAAA ATOM 2880 CB VAL 360 9.300 35.188 71.621 1.00 26.71 AAAA ATOM 2881 CG1 VAL 360 9.783 33.917 70.912 1.00 20.64 AAAA ATOM 2882 CG2 VAL 360 10.486 36.038 72.113 1.00 25.79 AAAA ATOM 2883 C VAL 360 7.228 35.202 70.197 1.00 25.51 AAAA ATOM 2888 N ARG 361 7.065 35.094 68.87 1.00 19.75 AAAA ATOM 2886 CA ARG 361 7.065 35.094 68.87 1.00 19.75 AAAA ATOM 2886 CA ARG 361 5.947 34.337 68.3C 1.00 22.01 AAAA ATOM 2887 CB ARG 361 5.948 34.389 66.772 1.00 19.31 AAAA ATOM 2888 CG ARG 361 5.446 35.671 66.204 1.00 30.86 AAAA ATOM 2889 CD ARG 361 5.446 35.671 66.204 1.00 30.86 AAAA ATOM 2889 CD ARG 361 7.111 36.148 64.460 1.00 30.73 AAAA ATOM 2891 CZ ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2891 CZ ARG 361 7.616 36.275 63.242 1.00 22.89 AAAA ATOM 2893 NH2 ARG 361 6.851 36.006 62.186 1.00 19.02 AAAA ATOM 2894 C ARG 361 5.897 32.879 68.714 1.00 26.11 AAAA ATOM 2894 C ARG 361 5.897 32.879 68.714 1.00 22.179 AAAA ATOM 2895 O ARG 361 5.897 32.879 68.714 1.00 22.91 AAAA ATOM 2895 C ARG 361 5.897 32.879 68.714 1.00 22.91 AAAA ATOM 2897 CA LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2899 CG LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 50.87 AAAA ATOM 2901 CE LYS 362 2.290 32.715 70.157 1.00 50.87 AAAA ATOM 2901 CE LYS 362 2.307 34.683 68.791 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 50.87 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2900 CD LYS 362 2.307 34.683 68.711 1.00 22.99 AAA | | | | | | | | | 69.449 | 1.00 | 22.94 | | AAAA |
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| ATOM 2893 NH2 ARG 361 8.861 36.704 63.081 1.00 23.47 AAAA ATOM 2894 C ARG 361 5.897 32.879 68.714 1.00 26.11 AAAA ATOM 2895 O ARG 361 6.926 32.255 68.968 1.00 21.79 AAAA ATOM 2896 N LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.479 30.938 69.125 1.00 28.63 AAAA ATOM 2898 CB LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | | | | | | | 36 006 | | | | | |
| ATOM 2894 C ARG 361 5.897 32.879 68.714 1.00 26.11 AAAA ATOM 2895 O ARG 361 6.926 32.255 68.968 1.00 21.79 AAAA ATOM 2896 N LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.479 30.938 69.125 1.00 28.63 AAAA ATOM 2898 CB LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2900 CD LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | | | | | | | | | | | | |
| ATOM 2895 O ARG 361 6.926 32.255 68.968 1.00 21.79 AAAA ATOM 2896 N LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.479 30.938 69.125 1.00 28.63 AAAA ATOM 2898 CB LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CD LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | | | | | | | | | | | | |
| ATOM 2896 N LYS 362 4.681 32.338 68.763 1.00 24.89 AAAA ATOM 2897 CA LYS 362 4.479 30.938 69.125 1.00 28.63 AAAA ATOM 2898 CB LYS 362 2.981 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | | | | | | | | | | | | |
| ATOM 2897 CA LYS 362 4.479 30.938 69.125 1.00 28.63 AAAA ATOM 2898 CB LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | | | | | | | | | | | | |
| ATOM 2898 CB LYS 362 2.961 30.570 69.070 1.00 22.91 AAAA ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | | | | | | | | | | | | |
| ATOM 2899 CG LYS 362 2.145 31.200 70.168 1.00 50.86 AAAA ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | ATOM | | | | | | | | | | | | |
| ATOM 2900 CD LYS 362 2.290 32.715 70.157 1.00 57.51 AAAA ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | ATOM | | | | | | 2.145 | | | | | | |
| ATOM 2901 CE LYS 362 1.923 33.278 68.799 1.00 50.87 AAAA ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | MOTA | | | | | | | | | | | | |
| ATOM 2902 NZ LYS 362 2.307 34.683 68.711 1.00 22.99 AAAA ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | ATOM | 2901 | | | | | 1.923 | | | | * | | |
| ATOM 2903 C LYS 362 5.269 30.014 68.202 1.00 16.77 AAAA | | 2902 | | | 362 | | | | | 1.00 | 22.99 | | |
| ATOM 2904 O LYS 362 5.808 29.007 68.647 1.00 22.90 AAAA | | | | | | | | | | 1.00 | 16.77 | | |
| | ATOM | 2904 | 0 | LYS | 362 | | 5.808 | 29.007 | 68.647 | 1.00 | 22.90 | | AAAA . |

| | | | | | • | | | | |
|--------|--------|-----|------------|------|--------|--------|---------|-------------------------|--------|
| * 500 | 2905 | N.T | GLU | 363 | 5.311 | 30.355 | 66.913 | 1.00 25.24 | AAAA |
| ATOM | | N | | | | 29.577 | 65.910 | 1.00 26.29 | AAAA |
| MOTA | 2906 | CA | GLU | 363 | 6.055 | | | | AAAA |
| ATOM | 2907 | CB | GLU | 363 | 6.207 | 30.342 | 64.608 | 1.00 33.50 | |
| ATOM | 2908 | CG | GLU | 363 | 4.999 | 30.639 | 63.824 | 1.00 48.73 | AAAA |
| | | | GLU | 363 | 5.368 | 31.494 | 62.638 | 1.00 42.01 | AAAA |
| MOTA | 2909 | CD | | | | 31.087 | 61.895 | 1.00 28.50 | AAAA |
| ATOM - | 2910 | | GLU | 363 | 6.299 | | | - | |
| ATOM | 2911 | OE2 | GLU | 363 | 4.738 | 32.558 | 62.461 | 1.00 44.91 | AAAA |
| | | | GLU | 363 | 7.481 | 29.326 | 66.349 | 1.00 19.00 | AAAA |
| MOTA | 2912 | С | | | | 28.218 | 66.226 | 1.00 18.66 | AAAA |
| MOTA | 2913 | 0 | GLU | 363 | 8.011 | | | • | |
| ATOM | 2914 | N | VAL | 364 | 8.121 | 30.399 | 66.790 | 1.00 20.69 | AAAA |
| | | | | 364 | 9.501 | 30.303 | 67.219 | 1.00 23.13 | AAAA |
| MOTA | 2915 | CA | VAL | | | 31.681 | 67.510 | 1.00 16.98 | AAAA |
| MOTA | 2916 | CB | VAL | .364 | 10.096 | | | | |
| ATOM | 2917 | CG1 | VAL | 364 | 11.515 | 31.513 | 68.010- | | AAAA |
| | | | VAL | 364 | 10.082 | 32.548 | 66.242 | 1.00 23.99 | AAAA |
| MOTA | 2918 | | | | 9.625 | 29.415 | 68.448 | 1.00 19.28 | AAAA |
| ATOM | 2919 | C, | VAL | 364 | | | | | - AAAA |
| ATOM | 2920 | 0 | VAL | 364 | 10.507 | 28.548 | 68.510· | | |
| | 2921 | N | LYS | 365 | 8.735 | 29.600 | 69.417 | 1.00 21.11 | AAAA |
| MOTA | | | | | 8.780 | 28.768 | 70.612 | 1.00 18.15 | AAAA |
| MOTA | 2922 | CA | LYS | 365 | | | | 1.00 25.22 | AAAA |
| MOTA | 2923 | CB | LYS | 365 | 7.711 | 29.210 | 71.626 | | |
| | 2924 | CG | LYS | 365 | 7.921 | 30.611 | 72.167 | 1.00 32.99 | AAAA |
| MOTA | | | | 365 | 6.901 | 30.949 | 73.253 | 1.00 36.09 | AAAA |
| MOTA | 2925 | CD | LYS | | | 32.357 | 73.790 | 1.00 28.99 | AAAA |
| MOTA | 2926 | CE | LYS | 365 | 7.121 | | | | |
| ATOM | 2927 | NZ | LYS | 365 | 6.178 | 32.736 | 74.882 | 1.00 38.98 | AAAA |
| | 2928 | C | LYS | 365 | 8.574 | 27,305 | 70.236 | 1.00 19.49 | AAAA |
| MOTA | | | | | 9.255 | 26.417 | 70.758 | 1.00 22.04 | AAAA |
| MOTA | 2929 | 0 | LYS | 365 | | | | 1.00 22.45 | AAAA |
| ATOM | 2930 | N | ASP | 366 | 7.635 | 27.048 | 69.327 | | |
| ATOM | 2931 | CA | ASP | 366 | 7.386 | 25.669 | 68.915 | 1.00 22.62 | AAAA |
| | | | | 366 | 6.173 | 25.574 | 67.967 | 1.00 21.69 | AAAA |
| ATOM | 2932 | CB | ASP | - | | 25.987 | 68.634 | 1.00 27.75 | AAAA |
| ATOM | 2933 | CG | ASP | 366 | 4.870 | | | | AAAA |
| MOTA | 2934 | OD1 | ASP | 366 | 4.763 | 25.890 | 69.881 | 1.00 31.01 | |
| | 2935 | | ASP | 366 | 3.938 | 26.382 | 67.907 | 1.00 33.20 | AAAA |
| MOTA | | | | | 8.606 | 25.034 | 68.237 | 1.00 24.53 | AAAA |
| MOTA | 2936 | С | ASP | 366 | | 23.871 | 68.480 | 1.00 21.13 | AAAA |
| ATOM | 2937 | 0 | ASP | 366 | 8.924 | | | | AAAA |
| ATOM | 2938 | N | THR | 367 | 9.281 | 25.787 | 67.380 | 1.00 26.19 | |
| | 2939 | ĊA | THR | 367 | 10.462 | 25.252 | 66.694 | 1.00 21.68 | AAAA |
| MOTA | | | | | 11.035 | 26.301 | 65.742 | 1.00 14.56 | AAAA |
| ATOM | 2940 | CB | THR | 367 | | | 64.697 | 1.00 21.76 | AAAA |
| ATOM | 2941 | OG1 | THR | 367 | 10.085 | 26.545 | | | |
| ATOM | 2942 | CG2 | THR | 367 | 12.340 | 25.825 | 65.138 | 1.00 19.83 | AAAA |
| | | | THR | 367 | 11.523 | 24.822 | 67.710 | 1.00 19.02 | AAAA |
| MOTA | 2943 | С | | | 12.071 | 23.717 | 67.625 | 1.00 21.79 | AAAA |
| ATOM | . 2944 | 0 | THR | 367 | | | | 1.00 18.42 | AAAA |
| ATOM | 2945 | N | LEU | 368 | 11.802 | 25.684 | 68.683 | | |
| | 2946 | CA | LEU | 368 | 12.797 | 25.348 | 69.700 | 1.00 21.02 | AAAA |
| ATOM | | | | 368 | 13.148 | 26.569 | 70.560 | 1.00 17.34 | AAAA |
| ATOM | 2947 | CB | LEU | | | 27.518 | 69.959 | 1.00 17.45 | AAAA |
| MOTA | 2948 | CG | LEU | 368 | 14.206 | | | 1.00 16.83 | AAAA |
| ATOM | 2949 | CD1 | LEU | 368 | 15.525 | 26.758 | 69.817 | | |
| | 2950 | | LEU | 368 | 13.756 | 28.041 | 68.593 | 1.00 19.49 | AAAA |
| ATOM | | | | | 12.361 | 24.189 | 70.589 | 1.00 23.17 | Aaaa |
| ATOM | 2951 | J | LEU | 368 | | | | 1.00 24.81 | AAAA |
| ATOM | 2952 | U | LEU | 368 | 13.203 | 23.420 | | | AAAA |
| ATOM | 2953 | И | GLU | 369 | 11.059 | 24,055 | 70.839 | 1.00 23.97 | |
| | | CA | GLU | 369 | 10.597 | 22.929 | 71.653 | 1.00 19.36 [,] | AAAA |
| MOTA | 2954 | | | | | 23.113 | 72.063 | 1.00 21.81 | AAAA |
| MOTA | 2955 | CB | GLU | 369 | 9.127 | | | | AAAA |
| MOTA | 2956 | CG | GLU | 369 | 8.913 | 24.225 | 73.100 | 1.00 40.15 | |
| | 2957 | CD | GLU | 369 | 7.450 | 24.416 | 73.487 | 1.00 49.38 | AAAA |
| MOTA | | | | | 6.806 | | | 1.00 43.26 | AAAA |
| MOTA | 2958 | | GLU | 369 | | | | 1.00 57.31 | AAAA |
| ATOM | 2959 | OE2 | GLU | 369 | 6.948 | | | | |
| | 2960 | С | GLU | 369 | 10.778 | | | 1.00 24.29 | AAAA |
| ATOM | | | | 369 | 11.172 | | 71.420 | 1.00 25.96 | AAAA |
| ATOM | 2961 | 0 | GLU | | 10.488 | | | | Aaaa |
| MOTA | 2962 | N | LYS | 370 | | | | 1.00 23.19 | AAAA |
| ATOM | 2963 | CA | LYS | 370 | 10.665 | | | | |
| | 2964 | | LYS | 370 | 10.051 | 20.596 | 67.347 | | AAAA |
| MOTA | | | | | 8.537 | | | 1.00 36.68 | AAAA |
| ATOM | 2965 | CG | LYS | 370 | | | | | AAAA |
| MOTA | 2966 | CD | LYS | 370 | 8.056 | | | | AAAA |
| MOTA | 2967 | CE | LYS | 370 | 6.567 | 20.105 | 65.740 | | |
| | | | | 370 | 6.082 | | | 1.00 56.10 | AAAA |
| ATOM | 2968 | NZ | LYS | | | | | | AAAA |
| MOTA | 2969 | С | LYS | 370 | 12.148 | 20.123 | | | AAAA |
| MOTA | 2970 | 0 | LYS | 370 | 12.549 | 18.958 | 68.587 | 1.00 20.00 | |
| TION | | Ť. | | • | | | | • | • |
| • | | | | | | | | | |

64/263 Figure 16-46

| ATOM | . 297 | 1 N | ALA | 371 | 12.9 | 161 21 1 | 30 60 40 | | | |
|--------|--------|--------|------------|------------|---------|------------------|------------------|-------|---------|--------------|
| ATOM | 297 | | | 371 | 14.4 | | | | 0 26.25 | |
| MOTA | 297 | | | 371 | 15.0 | | | | 0 27.33 | |
| ATOM | 297 | | ALA | 371 | 14.9 | | | | 0 23.70 | AAAA |
| ATOM | 297 | | ALA | 371 | | | | | 0 26.74 | |
| ATOM | 297 | | ALA | 372 | 15.8 | _ | | | 0 29.52 | |
| MOTA | 297 | | ALA | 372 372 | 14.4 | | | | 0 24.83 | |
| ATOM | 297 | | ALA | | 14.9 | | | | 0 34.24 | AAAA |
| ATOM | 297 | | ALA | 372 | 14.3 | | | | 0 37.17 | AAAA |
| MOTA | 298 | | | 372 | 14.6 | | | 1.0 | 0 45.62 | AAAA |
| ATOM | 298 | | ALA | 372 | 15.5 | | | | 0 35.52 | AAAA |
| MOTA | 298 | | ALĄ | 373 | 13.3 | | | | 0 44:50 | AAAA |
| MOTA | | _ | ALA | 373 | 13.0 | | | 2 1.0 | 0 49.88 | AAAA |
| | 298 | | ALA | 373 | 11.5 | | | | 0 49.32 | AAAA |
| MOTA | 298 | _ | ALA | 373 | 13.8 | | | | 0 44.64 | AAAA |
| ATOM | 298 | _ | ALA | 373 | 14.6 | | 0 71.201 | | 58.19 | AAAA |
| ATOM | 2986 | | ALA | 373 | 13.5 | | 7 69.626 | 1.00 | 41.63 | AAAA |
| | M 298 | | TAW | `1 | 36.3 | 68 43.90 | 7 49.242 | | 13.03 | SOLV |
| | M 2988 | | WAT | 2 | 23.1 | 07 30.58 | 4 59.802 | | 11.42 | SOLV |
| | M 2989 | | WAT | 3 | 20.5 | 94 33.74 | | | 14.73 | SOLV |
| | M 2990 | | WAT | 4 | 31.3 | 59 16.55 | | | 19.84 | SOLV |
| | M 2991 | | WAT | 5 | 30.38 | 39 18.14 | | | 19.94 | SOLV |
| | M 2992 | | TAW | 6 | 16.92 | 25 41.74 | | | 13.33 | |
| | M 2993 | | WAT | 7 | 28.44 | | 4 62.316 | | 14.08 | SOLV |
| HETAT | | | WAT | 8 | 40.37 | | | | 19.10 | SOLV |
| HETATI | | | WAT | 9 | 18.45 | 5 29.66 | | | 18.81 | SOLV |
| HETATI | M 2996 | OH2 | WAT | 10 | 26.30 | | | | 16.65 | SOLV |
| HETATI | | | WAT | 11 | 50.14 | | | | 16.53 | SOLV |
| HETATI | M 2998 | OH2 | WAT | 12 | 45.93 | | | | 25.08 | SOLV |
| HETATI | | | WAT | 13 | 26.35 | | | | 22.91 | SOLV |
| HETATI | 4 3000 | OH2 | WAT | 14 | . 48.72 | | | | 25.49 | SOLV |
| HETATI | 4 3001 | OH2 | WAT | 15 | 30.24 | | | | 25.78 | SOLV |
| HETATY | 4 3002 | OH2 | WAT | 16 | 10.61 | | | | 22.40 | SOLV |
| HETATI | 1 3003 | OH2 | WAT | 17 | 18.40 | | | | 21.46 | SOLV |
| HETATM | 1 3004 | OH2 | WAT | 18 | 22.19 | | | | 26.19 | SOLV |
| HETATM | 1,3005 | OH2 | WAT | 19 | 3.27 | | | | 20.19 | SOLV |
| HETATM | 3006 | · OH2 | WAT | 20 | 23.64 | | 59.512 | | 21.27 | SOLV |
| HETATM | 3007 | OH2 | WAT | 21 | 50.28 | | | | 19.73 | SOLV |
| HETATM | 3008 | OH2 | TAW | 22 | 44.72 | | | | 18.74 | SOLV |
| HETATM | | OH2 | | 23 | 8.34 | | | | 22.33 | SOTA |
| HETATM | | OH2 | TAW | 24 | 39.85 | | | | 20.43 | SOLV |
| HETATM | | OH2 | WAT | 25 | 7.82 | | | | 19.24 | SOLV |
| HETATM | | OH2 | WAT | 26 | 45.38 | | | | 20.86 | SOLV |
| HETATM | 3013 | OH2 | WAT | 27 | 47.63 | | | | 20.41 | SOLV |
| HETATM | 3014 | OH2 | TAW | 28 | 32.51 | | | | 24.76 | SOLV |
| HETATM | | OH2 | WAT | 29 | 26.18 | | | | 19.63 | SOLV |
| HETATM | | OH2 | TAW | 30 | 14.95 | | | | 23.80 | SOLV |
| HETATM | 3017 | OH2 | WAT | 31 | 24.483 | | | | 27.25 | SOLV |
| HETATM | 3018 | OH2 1 | TAW | 32 | 41.141 | | | | 25.99 | SOLV |
| HETATM | 3019 | OH2 | TAN | 33 | 23.104 | | | | 26.37 | SOLV |
| HETATM | | OH2 V | TAN | 34 | 51.301 | | | | 32.78 | SOLV |
| HETATM | 3021 | OH2 | TAV | 35 | 51.376 | | 53.156 | 1 00 | 24 27 | |
| HETATM | 3022 | OH2 Y | TAV | 36 | 12.518 | | 49.816 | | 23.60 | SOLV |
| HETATM | 3023 | OH2 V | TAV | 3 7 | 6.521 | | 50.861 | | 25.87 | SOLV |
| HETATM | 3024 | OH2 V | | 38 | 30.390 | | 34.190 | | 19.87 | SOLV SOLV |
| HETATM | 3025 | OH2 W | | 39 | 8.328 | | 62.062 | 1.00 | 32.01 | |
| HETATM | 3026 | OH2 W | | 40 | 30.180 | | 30.724 | 1.00 | 22.61 | SOLV |
| HETATM | 3027 | OH2 W | | 41 | 44.521 | | | | | SOLV |
| HETATM | • | OH2 W | | 42 | 30.981 | | 38.395 41.186 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 43 | 14.632 | | 73.830 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 44 | 39.332 | | 73.830 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 45 | 7.597 | 37.592 | | 1.00 | | SOLV |
| HETATM | | OH2 W | | 46 | 15.027 | 18.079 | 51.896 54.822 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 47 | 11.076 | 45.493 | 54.827 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 48 | 42.124 | | 66.435 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 49 | 48.736 | 18.055 25.764 | 37.233 | 1.00 | | SOLV |
| HETATM | | OH2 W | | 50 | 50.383 | | 64.149 | 1.00 | | SOLV |
| | | VIIZ W | ur 1 | | 20.303 | 27.254 | 54.972 | 1.00 | 24.36 | SOLV |

| HETATM 303 | 7 OH2 WAT | 51 | 48.659 | 36.025 | 68.226 | 1.00 33.89 | SOLV |
|-------------|-------------|------|--------|--------|--------|-------------|------|
| | | | 36.998 | 27.228 | 71.440 | 1.00 21.03 | SOLV |
| HETATM 303 | | | | | | 1.00 32.23 | SOLV |
| нетатм 303 | 9 OH2 WAT | 53 | 41.303 | 16.309 | 55.307 | | |
| HETATM 304 | O OH2 WAT | 54 | 33.242 | 39.524 | 49.454 | 1.00 29.77 | SOLV |
| HETATM 304 | 11 OH2 WAT | 55 | 45.004 | 25.973 | 35.031 | 1.00 21.59 | SOLV |
| HETAIM 30 | I OHE WAL | | | | 45.793 | 1.00 33.48 | SOLV |
| HETATM 304 | 12 OH2 WAT | 56 | 19.039 | 25.829 | | | |
| HETATM 304 | 3 OH2 WAT | 57 | 17.922 | 35.542 | 50.154 | 1.00 37.51 | SOLV |
| | | 58 | 10.409 | 26.864 | 73.166 | 1.00 26.54 | SOLV |
| HETATM 304 | | | | | | | SOLV |
| HETATM 304 | 15 OH2 WAT | 59 | 11.835 | 22.805 | 59.408 | 1.00 20.83 | |
| HETATM 304 | | 60. | 18.254 | 48.699 | 53.224 | 1.00 28.41 | SOLV |
| | | 61 | 10.426 | 26.647 | 60.447 | 1.00 32.72 | SOLV |
| HETATM 304 | | | | | | | SOLV |
| HETATM 304 | 18 OH2 WAT | 62 | 21.304 | 55.086 | 63.510 | 1.00 28.84 | |
| HETATM 304 | 9 OH2 WAT | 63 | 32.532 | 51.211 | 45.469 | 1.00 32.48 | SOĻV |
| | | 64 | 22.658 | 61.079 | 57.420 | 1.00 27.32 | SOLV |
| HETATM 30 | | | | | 74.721 | 1.00 27.44 | SOLV |
| HETATM 305 | on2 wat | 65 | 16.734 | 24.334 | | | |
| HETATM 305 | 2 OH2 WAT | 66 | 32.758 | 37.824 | 54.391 | 1.00 25.07 | SOLV |
| | | 67 | 11.142 | 25.859 | 49.706 | 1.00 29.66 | SOLV |
| HETATM 30 | _ | | | 15.261 | 53.236 | 1.00 30.21 | SOLV |
| HETATM 305 | 4 OH2 WAT | 68 | 24.192 | | | | |
| HETATM 305 | 55 OH2 WAT | 69 | 19.816 | 17.916 | 66.357 | 1.00 30.50 | SOLV |
| HETATM 305 | | 70 | 50.347 | 23.975 | 53.197 | 1.00 28.08 | SOLV |
| | | | 50.258 | 30.918 | 51.113 | 1.00 20.19 | SOLV |
| HETATM 305 | | 71 | | | | | |
| HETATM 305 | 8 OH2 WAT | 72 | 21.047 | 17.624 | 68.693 | 1.00 41.23 | SOLV |
| HETATM 305 | | 73 | 26.782 | 33.756 | 49.995 | 1.00 25.80 | SOLV |
| | | | 12.570 | 43.844 | 64.441 | 1.00 31.03 | SOLV |
| HETATM 306 | | 74 | | | | | |
| HETATM 306 | 51 OH2 WAT | 75 | 35.555 | 41.287 | 50.852 | 1.00 24.03 | SOLV |
| HETATM 306 | | 76 | 27.764 | 18.231 | 61.827 | 1.00 18.28 | SOLV |
| | | 77 | 26.715 | 29.236 | 38.391 | 1.00 23.18 | SOLV |
| HETATM 306 | 3 OH2 WAT | | | | | 1.00 23.80 | SOLV |
| HETATM 306 | 64 OH2 WAT | 78 | 21.461 | 23.245 | 48.872 | | |
| HETATM 306 | 55 OH2 WAT | 79 | 49.246 | 28.263 | 65.477 | 1.00 21.52 | SOLV |
| | | 80 | 31.785 | 13.301 | 69.606 | 1.00 31.11 | SOLV |
| HETATM 306 | | | | 34.740 | 59.229 | 1.00 31.76 | SOLV |
| HETATM 306 | 57 OH2 WAT | 81 | 49.811 | | | | |
| HETATM 306 | 8 OH2 WAT | 82 | 45.670 | 33.188 | 42.470 | 1.00 23.13 | SOLV |
| HETATM 306 | | 83 | 9.408 | 39.751 | 55.872 | 1.00 31.53 | SOLV |
| | | | | 35.878 | 29.899 | 1.00 37.32 | SOLV |
| нетатм 307 | 0 OH2 WAT | 84 | | | | 1.00 44.07 | SOLV |
| HETATM 307 | 11 OH2 WAT | 85 | 41.927 | 22.970 | 73.694 | • | |
| HETATM 307 | 2 OH2 WAT | 86 | 22.125 | 34.577 | 49.199 | 1.00 44.65 | SOLV |
| | | 87 | 43.984 | 33.541 | 37.965 | 1.00 24.88 | SOLV |
| HETATM 307 | OHZ WAI | | | 17.962 | 56.312 | 1.00 34.85 | SOLV |
| HETATM 307 | 4 OH2 WAT | 88 | 11.997 | | | | |
| HETATM 307 | 75 OH2 WAT | 89 | 42.194 | 14.737 | 59.766 | 1.00 25.91 | SOLV |
| HETATM 307 | | 90 | 49.313 | 24.200 | 41.684 | 1.00 29.29 | SOLV |
| | | 91 | 48.504 | 33.595 | 61.519 | 1.00 30.32 | SOLV |
| HETATM 307 | | | | | | 1.00 53.13 | SOLV |
| HETATM 307 | 78 OH2 WAT | 92 | 24.773 | 18.356 | 33.365 | | |
| HETATM 307 | | 93 | 35.160 | 35.656 | 47.470 | 1.00 41.41 | SOLV |
| | | 94 | 44.682 | 36.658 | 39.962 | 1.00 29.24 | SOLV |
| HETATM 308 | | | 9.576 | 41.033 | 52.549 | 1.00 51.83 | SOLV |
| HETATM 308 | 31 OH2 WAT | 95 | | | | | SOLV |
| HETATM 308 | 32 OH2 WAT | ^6 | 47.199 | 20.112 | 42.102 | 1.00 40.39 | |
| HETATM 308 | | 7ر ٠ | 49.254 | 26.331 | 59.641 | 1.00 37.03 | SOLV |
| MEININ 300 | 4 0110 1130 | _8 | 26.808 | 37.600 | 38.172 | 1.00 28.74 | SOLV |
| HETATM 308 | | | | 14.572 | 64.635 | 1.00.33.42 | SOLV |
| HETATM 308 | 5 OH2 WAT | 99 | 40.749 | | | | |
| HETATM 308 | 6 OH2 WAT | 100 | 24.850 | 44.161 | 47.775 | 1.00 27.89 | SOLV |
| nginin 300 | | 101 | 34.326 | 42.063 | 46.714 | 1.00 42.22 | SOLV |
| HETATM 308 | Onz WAI | | 30.226 | 34.544 | 52.026 | 1.00 30.77 | SOLV |
| HETATM 308 | 8 OH2 WAT | 102 | | | | 1.00 50.17 | |
| HETATM 308 | 9 OH2 WAT | 103 | 47.824 | 39.054 | 78.097 | 1.00 52.16 | SOLV |
| HETATM 309 | O OH2 WAT | 104 | 19.665 | 18.953 | 47.438 | 1.00 51.70 | SOLV |
| HETAIM 303 | ONZ WAI | | 46.857 | 36.525 | 46.232 | 1.00 23.65 | SOLV |
| HETATM 309 | 1 OH2 WAT | 105 | | | | 1.00 37.56 | SOLV |
| HETATM 309 | 2 OH2 WAT | 106 | 48.069 | 19.460 | 67.360 | 1.00 37.30 | |
| HETATM 309 | | 107 | 15.553 | 56.850 | 61.838 | 1.00 46.95 | SOLV |
| | | 108 | 44.026 | 19.119 | 70.671 | 1.00 39.55 | SOLV |
| HETATM 309 | | | | | 65.674 | 1.00 42.61 | SOLV |
| HETATM 309 | 5 OH2 WAT | 109 | 8.139 | 42.064 | | T.00 35.05 | |
| HETATM 309 | 6 OH2 WAT | 110 | 50.624 | 36.591 | 65.779 | 1.00 31.59 | SOLV |
| UPINITE 303 | שאנה כמט שי | 111 | 51.398 | 26.073 | 61.043 | 1.00 49.09 | SOLV |
| HETATM 309 | 7 OH2 WAT | | 26.174 | 33.692 | 33.551 | 1.00 36.61 | SOLV |
| HETATM 309 | 8 OH2 WAT | 112 | | | | 1.00 24.34 | SOLV |
| HETATM 309 | 9 OH2 WAT | 113 | 23.545 | 20.203 | 53.001 | 1.00 24.34 | |
| HETATM 310 | O OH2 WAT | 114 | 9.083 | 42.965 | 57.697 | 1.00 33.65 | SOLV |
| WEININ 310 | | | 8.442 | 39.898 | 64.594 | 1.00 31.21 | SOLV |
| HETATM 310 | | 115 | | | | 1.00 26.59 | SOLV |
| HETATM 310 | 2 OH2 WAT | 116 | 15.219 | 35.897 | 51.951 | 1.00, 20.22 | |
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|--------------------|------------|-------|---------|------------------|--------|------------|--------|
| HETATM 31 | 03 OH2 WA7 | 117 | 15.417 | 7 38.438 | 50.473 | 1.00 34.46 | |
| HETATM 31 | 04 OH2 WAT | 118 | 40.757 | | | 1.00 34.40 | SOLV |
| HETATM 31 | | | | | | | SOLV |
| | | | 27.717 | | | | SOLV |
| HETATM 31 | | | 18.612 | ? 13.78 <i>6</i> | | 1.00 38.56 | SOLV |
| HETATM 31 | 07 OH2 WAT | 121 | 43.198 | 31.377 | | 1.00 26.31 | |
| HETATM 31 | 08 OH2 WAT | 122 | 44.188 | | | | SOLV |
| HETATM 31 | | | | | | | SOLV |
| | • | | 50.736 | | | | SOLV |
| HETATM 31: | | | 31.302 | 33.760 | 31.742 | 1.00 30.84 | SOLV |
| HETATM 31: | li oh2 wat | 125 | 36.895 | 21.264 | | | |
| HETATM 313 | 12 OH2 WAT | 126 | 47.474 | | | | SOLV |
| HETATM 313 | | | | | | | SOLV |
| | | | - 7.178 | | | | SOLV |
| HETATM 313 | | | 36.362 | | 54.021 | 1.00 36.88 | SOLV |
| HETATM 311 | | 129 | 42.486 | 35.503 | 30.348 | 1.00 26.61 | SOLV |
| HETATM 311 | 6 OH2 WAT | 130 | 8.432 | 34.383 | | 1.00 37.45 | |
| HETATM 311 | 7 OH2 WAT | | 37.644 | | | 1.00 37.43 | SOLV |
| HETATM 311 | | | | | 510 | | SOLV |
| | | | 50.273 | | | | SOLV |
| HETATM 311 | - | 133 | 7.518 | | | 1.00 45.42 | SOLV |
| HETATM 312 | | 134 | 31.483 | 46.197 | 72.538 | 1.00 28.02 | SOLV |
| HETATM 312 | 1 OH2 WAT | 135 | 41.501 | | | 1.00 32.78 | |
| HETATM 312 | 2 OH2 WAT | 136 | 45.898 | 47.740 | | | SOLV |
| HETATM 312 | | | | | | 1.00 43.47 | SOLV |
| | | 137 | 16.300 | 33.614 | 49.519 | 1.00 30.37 | SOLV |
| HETATM 312 | | 138 | 51.148 | 36.946 | 55.148 | 1.00 46.34 | SOLV |
| HETATM 312 | | 139 | 21.525 | 53.761 | 50.892 | 1.00 38.27 | SOLV |
| HETATM 312 | 6 OH2 WAT | 140 | 21.603 | 54.580 | 68.690 | 1.00 33.10 | |
| HETATM 312 | | 141 | 10.191 | 29.237 | | | SOLV |
| HETATM 312 | | | - | | 60.325 | 1.00 30.24 | SOLV |
| | | 142 | 16.951 | 18.120 | 66.901 | 1.00 40.85 | SOLV |
| HETATM 312 | | 143 | 4.943 | 24.912 | 51.199 | 1.00 49.13 | SOLV |
| HETATM 313 | O OH2 WAT | 144 | 10.711 | 25.291 | 58.177 | 1.00 30.72 | SOLV |
| HETATM 313. | 1 OH2 WAT | 145 | 30.815 | 43.398 | 36.040 | 1.00 42.23 | |
| HETATM 313 | CH2 WAT | 146 | 21.763 | 24.512 | | | SOLV |
| HETATM 313 | | | | | 46.695 | 1.00 28.31 | SOLV |
| | | | 51.788 | 33.122 | 50.887 | 1.00 26.15 | SOLV |
| HETATM 313 | | 148 | 24.531 | 44.741 | 72.420 | 1.00 27.99 | SOLV |
| HETATM 313 | 5 OH2 WAT | 149 | 50.938 | 23.483 | 60.422 | 1.00 38.20 | SOLV |
| HETATM 3136 | OH2 WAT | 150 | 24.860 | 47.932 | 61.067 | 1.00 18.89 | |
| HETATM 3137 | OH2 WAT | 151 | 27.336 | 37.304 | 35.642 | | SOLV |
| HETATM 3138 | | 152 | 38.680 | | 35.042 | 1.00 33.58 | SOLV |
| HETATM 3139 | | | | 35.535 | 35.974 | 1.00 26.89 | SOLV |
| | | 153 | 24.441 | 16.097 | 33.317 | 1.00 48.33 | SOLV |
| HETATM 3140 | | 154 | 20.343 | 18.124 | 73.416 | 1.00 36.28 | SOLV |
| HETATM 3141 | | 155 | 49.765 | 37.948 | 74.801 | 1.00 48.41 | SOLV |
| HETATM 3142 | OH2 WAT | 156 | 34.329 | 31.169 | 47.547 | 1.00 25.33 | |
| HETATM 3143 | OH2 WAT | 157 | 43.028 | 24.554 | | | SOLV |
| HETATM 3144 | | 158 | | | 72.536 | 1.00 41.54 | SOLV |
| | | | 39.888 | 15.082 | 42.035 | 1.00 28.76 | SOLV |
| HETATM 3145 | | 159 | 41.886 | 20.780 | 73.179 | 1.00 51.03 | SOLV |
| HETATM 3146 | | 160 | 22.962 | 49.969 | 58.518 | 1.00 35.04 | SOLV |
| HETATM 3147 | | 161 | 14.696 | 15.261 | 68.016 | 1.00 55.47 | SOLV |
| HETATM 3148 | OH2 WAT | 162 | 14.915 | 18.181 | 64.866 | 1.00 42.00 | |
| HETATM 3149 | | 163 | 30.608 | 49.029 | | | . SOLV |
| HETATM 3150 | | | | | 52.612 | 1.00 47.32 | . SOLV |
| | | 164 | 52.566 | 30.906 | 57.612 | 1.00 36.71 | SOLV |
| HETATM 3151 | OH2 WAT | 165 | 23.699 | 27.331 | 77.729 | 1.00 32.22 | SOLV |
| HETATM 3152 | OH2 WAT | 166 | 36.971 | 59.046 | 63.272 | 1.00 43.05 | SOLV |
| HETATM 3153 | OH2 WAT | 167 | 46.053 | 45.927 | 52.876 | 1.00 33.66 | SOLV |
| HETATM 3154 | OH2 WAT | 168 | 42.780 | 49.151 | | | |
| HETATM 3155 | OH2 WAT | 169 | | | | 1.00 44.63 | SOLV |
| | | | 15.100 | 44.506 | 72.183 | 1.00 45.43 | SOLV |
| HETATM 3156 | OH2 WAT | 170 | 31.677 | 60.99B· | 50.050 | 1.00 34.51 | SOLV |
| HETATM 3157 | OH2 WAT | 171 | 25.336 | 45.674 | 45.578 | 1.00 55.85 | SOLV |
| HETATM 3158 | OH2 WAT | 172 | 17.481 | 18.266 | 49:018 | 1.00 32.73 | SOLV |
| HETATM 3159 | OH2 WAT | 173 | 26.112 | 18.147 | 31.404 | | |
| HETATM 3160 | OH2 WAT | | | | | 1.00 49.94 | SOLV |
| | | 174 . | 45.874 | 43.142 | 70.985 | 1.00 32.89 | SOLV |
| HETATM 3161 | OH2 WAT | 175 | 34.517 | 17.884 | 33.278 | 1.00 42.20 | SOLV |
| HETATM 3162 | OH2 WAT | 176 | 16.330 | 54.886 | 50.466 | 1.00 40.74 | SOLV |
| HETATM 3163 | OH2 WAT | 177 | 31.400 | 51.087 | 74.689 | 1.00 38.56 | SOLV |
| HETATM 3164 | OH2 WAT | 178 | | 27.079 | 67.130 | 1.00 44.49 | |
| HETATM 3165 | OH2 WAT | 179 | | 23.412 | | | SOLV |
| | | | | | 54.691 | 1.00 42.84 | SOLV |
| HETATM 3166 | OH2 WAT | 180 | | 47.596 | 73.612 | 1.00 35.99 | SOLV |
| HETATM 3167 | OH2 WAT | 181 | | 19.583 | 44.954 | 1.00 51.31 | SOLV |
| HETATM 3168 | OH2 WAT | 182 | 40.139 | 17.026 | 74.920 | 1.00 43.64 | SOLV |
| | | • | | - | | | |

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| | | | | | | | | 1 00 24 51 | SOLV |
|--------|--------|------|------------|-----|--------|--------|---------|------------|--------|
| HETATM | 3169 | OH2 | TAW | 183 | 10.441 | 42.659 | 62.744 | 1.00 34.51 | SOLV |
| HETATM | 3170 | OH2 | WAT | 184 | 2.095 | 34.482 | 65.810 | 1.00 36.49 | SOLV |
| HETATM | 3171 | OH2 | | 185 | 45.749 | 18.286 | 51.615 | 1.00 28.19 | |
| HETATM | 3172 | OH2 | | 186 | 25.771 | 38.332 | 76.707 | 1.00 45.53 | SOLV |
| HETATM | 3173 | OH2 | | 187 | 7.228 | 40.382 | 57.542 | 1.00 48.91 | SOLV |
| HETATM | 3174 | OH2 | | 188 | 42.972 | 52.824 | 67.739 | 1.00 39.99 | SOLV |
| HETATM | 2175 | OH2 | | 189 | 20.137 | 13.189 | 73.277 | 1.00 44.91 | SOLV |
| HETATM | 2175 | OH2 | | 190 | 48.945 | 19.193 | 47.581 | 1.00 52.88 | SOLV |
| HETATM | 3170 | OH2 | | 191 | 14.549 | 34.547 | 47.665 | 1.00 49.15 | SOLV |
| HETATM | 3177 | | WAT | 192 | 31.765 | 20.567 | 26.536 | 1.00 42.23 | SOLV |
| HETATM | 3170 | | WAT | 193 | 9.784 | 39.303 | 74.222 | 1.00 32.10 | SOLV |
| HETATM | 31/9 | | WAT | 194 | 28.865 | 12.481 | 52.375 | 1.00 50.98 | SOLV |
| HEŢATM | 3180 | | WAT | 195 | 24.030 | 12.804 | 70.409- | 1.00 52.43 | SOLV |
| HETATM | 3191 | | WAT | 196 | 47.209 | 39.53€ | 50.698 | 1.00 43.03 | SOLV |
| HETATM | 3182 | | WAT | 197 | 35.618 | 18.114 | 27.306 | 1.00 41.11 | SOLV |
| HETATM | 3183 | | WAT | 198 | 23.625 | 48.145 | 43.853 | 1.00 48.20 | SOLV |
| HETATM | 3184 | | WAT | 199 | 37.090 | 59.044 | 54.185 | 1.00 34.99 | SOLV |
| HETATM | 3185 | | WAT | 200 | 34.478 | 12.208 | 59.080 | 1.00 36.58 | SOLV |
| HETATM | 3186 | | | 201 | 22.142 | 29.583 | 76.228 | 1.00 33.95 | SOLV |
| HETATM | 3187 | | WAT | 202 | 13.608 | 42.619 | 53.973 | 1.00 40.44 | SOLV |
| HETATM | 3188 | | WAT | 203 | 42.647 | 18.701 | 72.526 | 1.00 55.64 | SOLV |
| HETATM | 3189 | | WAT WAT | 204 | 37.005 | 35.993 | 77.480 | 1.00 34.82 | SOLV |
| HETATM | 3190 | | WAT | 205 | 34.154 | 20.512 | 33.327 | 1.00 31.00 | SOLV |
| HETATM | 3191 | | WAT | 205 | 37.264 | 57.546 | 47.642 | 1.00 49.58 | SOLV |
| HETATM | 3192 | | WAT | 207 | 17.924 | 35.195 | 79.003 | 1.00 38.45 | SOLV |
| HETATM | 3193 | | WAT | 208 | 51.172 | 31.581 | 62.378 | 1.00 35.37 | . SOLV |
| HETATM | 3194 | | WAI | 209 | 50.503 | 36.726 | 79.224 | 1.00 39.95 | SOLV |
| HETATM | 3195 | | | 210 | 18.382 | 13.162 | 63.852 | 1.00 52.08 | SOLV |
| HETATM | 3196 | | WAT WAT | 211 | 27.245 | 8.351 | 55.199 | 1.00 39.12 | SOLV |
| HETATM | 3197 | | WAT | 212 | 18.354 | 13.545 | 59.540 | 1.00 30.15 | SOLV |
| HETATM | 3198 | | WAT | 213 | 49.088 | 51.744 | 63.388 | 1.00 36.69 | SOLV |
| HETATM | 3199 | | WAT | 214 | 23.251 | 33.160 | 50.871 | 1.00 42.11 | SOLV |
| HETATM | 3200 | | WAT | 215 | 12.989 | 35.073 | 50.651 | 1.00 38.63 | SOLV |
| HETATM | 3201 | OHZ | WAT | 216 | 24.414 | 44.460 | 43.239 | 1.00 37.93 | SOLV |
| HETATM | 3202 | | WAT | 217 | 24.690 | 47.590 | 73.117 | 1.00 34.17 | SOLV |
| HETATM | 3203 | | WAT | 218 | 19.844 | 17.949 | 81.360 | 1.00 40.74 | SOLV |
| HETATM | 3204 | ONZ | WAT | 219 | 40.169 | 27.215 | 74.247 | 1.00 37.83 | SOLV |
| HETATM | 3205 | | WAT | 220 | 38.737 | 39.516 | 73.171 | 1.00 49.20 | SOLV |
| HETATM | 3200 | | TAW | 221 | 50.628 | 21.408 | 46.879 | 1.00 45.57 | SOLV |
| HETATM | 3207 | 002 | WAT | 222 | 35.436 | 43.288 | 75.660 | 1.00 37.33 | SOLV |
| HETATM | 3208 | OUZ | WAT | 223 | 34.390 | 16.963 | 55.285 | 1.00 35.10 | SOLV |
| HETATM | 3209 | 2072 | WAT | 224 | 21.800 | 35.454 | | 1.00 46.29 | SOLV |
| HETATM | 3210 | | WAT | 225 | 15.751 | 40.989 | | 1.00 62.75 | SOLV |
| HETATM | 1 2217 | | WAT | 226 | 23.844 | 48.662 | 66.295 | 1.00 38.35 | SOLV |
| HETATM | 3212 | | WAT | 227 | 47.225 | 20.562 | | 1.00 49.99 | SOLV |
| HETATM | 3213 | | TAK | 228 | 23.426 | 19.272 | 50.565 | 1.00 30.07 | SOLV |
| HETATM | 1 3214 | UHZ | AM. | 220 | | | | | - |

| | n | 7 7 | | _ | | |
|--------------|-----------------------------|--------|------------------|------------------|------------|---------|
| MOM. | Residu | | Y | Z | OCC. B | Segment |
| MOTA | 1 CB ALA A 2 2 C ALA A 2 | 43.739 | | | | |
| MOTA | - | 44.405 | | | | |
| MOTA | | 43.251 | | | | |
| ATOM | 4 N ALA A 2 | 46.142 | | | | |
| MOTA | 5 CA ALA A 2 | 44.776 | | | | |
| ATOM | 6 N LYS A 3 | 45.398 | | 72.233 | 1.00 55.40 | 7 |
| APOM | 7 CA LYS A 3 | 45.196 | | | 1.00 53.02 | 6 |
| ATOM | 8 CB LYS A 3 | 46.443 | 39.830 | 70.421 | | |
| MOTA | 9 CG LYS A. 3 | 47.703 | 40.093 | 71.217 | | |
| ATOM | 10 CD LYS A 3 | 48.941 | 39.976 | 70.349 | | |
| ATOM . | 11 CE LYS A 3 | 48.909 | 40.957 | 69.196 | | |
| ATOM | 12 NZ LYS A 3 | 50.075 | | | | |
| ATOM | 13 C LYS A 3 | 43.986 | | 70.399 | | 6 |
| MOTA | 14 O LYS A 3 | 43.691 | | 70.063 | 1.00 52.50 | |
| ATOM | 15 N VAL A 4 | 43.281 | | 70.034 | 1.00 45.96 | 8 |
| MOTA | 16 CA VAL A 4 | 42.122 | | 69.167 | | 7 |
| ATOM | 17 CB VAL A 4 | 40.983 | 41.272 | 69.638 | 1.00 41.16 | |
| MOTA | 18 CG1 VAL A 4 | 39.734 | | | 1.00 41.53 | 6 |
| ATOM | 19 CG2 VAL A 4 | | 41.028 | 68.797 | 1.00 40.07 | 6 |
| | | 40.705 | 41.033 | 71.115 | 1.00 38.31 | - · |
| . ATOM | | 42.619 | 40.796 | 67.796 | 1.00 39.96 | 6 |
| ATOM. | | 43.123 | 41.914 | 67.645 | 1.00 39.15 | 8 |
| MOTA | 22 N LYS A 5 | 42.486 | 39.916 | 66.807 | 1.00 36.24 | 7 |
| MOTA | 23 CA LYS A 5 | 42.956 | 40.186 | 65.449 | 1.00 35.66 | 6 |
| ATOM | 24 CB LYS A 5 | 43.930 | 39.088 | 65.024 | 1.00 37.33 | 6 |
| ATOM | 25 CG LYS A 5 | 45.197 | 38.978 | 65.860 | 1.00 38.24 | 6 |
| ATOM | 26 CD LYS A 5 | 46.113 | 40.179 | 65.659 | 1.00 35.41 | 6 |
| ATOM | 27 CE LYS A 5 | 47.436 | 39.957 | 66.369 | 1.00 37.46 | 6 |
| MOTA | 28 NZ LYS A 5 | 48.345 | 41.121 | 66.245 | 1.00 35.63 | 7 |
| MOTA | 29 C LYS A 5 | 41.840 | 40.254 | 64.415 | 1.00 34.40 | 6 |
| MOTA | 30 O LYS A 5 | 40.788 | 39.641 | 64.588 | 1.00 33.92 | 8 |
| MOTA | 31 N LEUA 6 | 42.082 | 40.983 | 63.329 | 1.00 32.52 | 7 |
| MOTA | 32 CA LEU A 6 | 41.097 | 41.094 | 62.253 | 1.00 33.64 | 6 |
| MOTA | 33 CB LEU A 6 | 40.589 | 42.532 | 62.114 | 1.00 31.83 | 6 |
| MOTA | 34 CG LEUA 6 | 39.346 | 42.823 | 61.248 | 1.00 32.93 | 6 |
| MOTA | 35 CD1 LEU A 6 | 39.356 | 44.295 | 60.899 | 1.00 28.95 | 6 |
| ATOM | 36 CD2 LEU A 6 | 39.336 | 42.031 | 59.964 | 1.00 32.87 | 6 |
| MOTA | 37 C LEUA 6 | 41.802 | 40.721 | 60.955 | 1.00 35.09 | 6 |
| ATOM | 38 O LEUA 6 | 42.631 | 41.491 | 60.468 | 1.00 36.93 | 8 |
| MOTA | 39 N ILE A 7 | 41.494 | 39.561 | 60.382 | 1.00 35.52 | 7 |
| ATOM | 40 CA ILE A 7 | 42.145 | 39.199 | 59.129 | 1.00 35.14 | 6 |
| ATOM | 41 CB ILE A 7 | 42.062 | 37.711 | 58.850 | 1.00 33.68 | 6 |
| ATOM | 42 CG2 ILE A 7 | 42.731 | 37.409 | 57.517 | 1.00 33.00 | 6. |
| ATOM | 43 CG1 ILE A 7 | 42.746 | 36.941 | 59.975 | 1.00 33.32 | 6 |
| ATOM | 44 CD1 ILE A 7 | 42.744 | 35.451 | 59.755 | 1.00 35.09 | 6 |
| MOTA | 45 C ILE A 7 | 41.487 | 39.935 | 57.971 | 1.00 37.13 | |
| ATOM | 46 O ILE A 7 | 40.258 | 39.933 | 57.855 | | 6 |
| ATOM | 47 N GLY A 8 | 42.304 | 40.563 | | 1.00 35.21 | 8 |
| ATOM T | 48 CA GLY A 8 | 41.771 | 41.305 | 57.124 55.994 | 1.00 37.25 | . 7 |
| ATOM | 49 C GLY A 8 | 42.809 | | | 1.00 38.69 | 6 |
| ATOM | 50 O GLY A 8 | 44.015 | 41.939 41.827 | 55.079 | 1.00 39.73 | 6 |
| | | | | JJ.JLI | | 8 |
| ATOM ATOM | | 42.335 | | 54.033 | 1.00 39.41 | 7 |
| | = = | 43.212 | 43.268 | 53.057 | 1.00 38.69 | 6 . |
| MOTA | 53 CB THRA 9 | 44.132 | 42.210 | 52.390 | 1.00 37.27 | 6 |
| ATOM | 54 OG1 THR A 9 | 44.754 | 42.771 | 51.230 | 1.00 36.82 | 8 |
| ATOM | 55 CG2 THR A 9 | 43.332 | 40.972 | 52.001 | 1.00 38.59 | 6 |
| ATOM | 56 C THR A 9 | 42.447 | 44.045 | 51.970 | 1.00 38.60 | 6 |
| ATOM | 57 O THRA 9 | 41.434 | 43.569 | 51.452 | 1.00 37.30 | 8 |
| MOTA | 58 N LEUA 10 | 42.939 | 45.238 | 51.628 | 1.00 38.14 | 7 |
| MOTA | 59 CA LEU A 10 | 42.304 | 46.077 | 50.609 | 1.00 39.39 | 6 |
| ATOM | 60 CB LEU A 10 | 43.026 | 47.418 | 50.456 | 1.00 38.98 | 6 |
| ATOM | 61 CG LEU A 10 | 42.836 | 48.506 | 51.510 | 1.00 39.68 | 6 |
| ATOM | 62 CD1 LEU A 10 | 41.343 | 48.830 | 51.594 | 1.00 40.22 | 6 |
| ATOM | 63 CD2 LEU A 10 | 43.382 | | 52.857 | 1.00 40.11 | 6 |
| ATOM | 64 C LEU A 10 | 42.238 | | 49.239 | 1.00 41.66 | 6 |
| ATOM | 65 O LEU A 10 | 41.462 | | 48.381 | 1.00 42.08 | 8 |
| | 66 N ASP A 11 | 43.052 | | 49.025 | 1.00 43.51 | 7 |
| MOTA | | | 44.408 | | | |

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Figure 17-2

| | | | | | | | | | 1 00 47 37 | c |
|--------|-----|-------|-------|------|---|--------|---------|---------|-------------|----|
| ATOM | 67 | CA | ASP A | 11 | | 43.071 | 43.731 | 47.737 | 1.00 47.27 | 6 |
| | 68 | | ASP A | 11 | | 44.250 | 42.765 | 47.694 | 1.00 51.03 | 6 |
| MOTA | | | ASP A | 11 | | 45.579 | 43.479 | 47.858 | 1.00 54.10 | 6 |
| MOTA | 69 | | | | | 45.944 | 44.282 | 46.975 | 1.00 55.93 | 8 |
| ATOM | 70 | | ASP A | 11 | | | 43.251 | 48.879 | 1.00 57.79 | 8 |
| ATOM | 71 | OD2 | ASP A | 11 | | 46.255 | | | | 6 |
| ATOM | 72 | С | ASP A | 11 | | 41.756 | 43.016 | 47.423 | 1.00 46.36 | |
| ATOM | 73 | | ASP A | 11 | | 41.472 | 42.702 | 46.266 | 1.00 43.49 | 8 |
| | - | | TYR A | 12 | | 40.954 | 42.767 | 48.456 | 1.00 46.80 | 7 |
| ATOM | 74 | | | | | 39.654 | 427.116 | 48.284 | 1.00 45.92 | 6΄ |
| MOTA | 75 | | TYR A | 12 | | | 41.942 | 49.638 | 1.00 41.38 | 6 |
| ATOM | 76 | CB | TYR A | 12 | | 38.953 | | | 1.00 38.82 | 6 |
| MOTA | 77 | CG | TYR A | 12 | - | 39.358 | 40.697 | 50.390 | | |
| ATOM | 78 | CD1 | TYR A | 12 | | 39.531 | 40.720 | 51.775 | 1.00 37.95 | 6 |
| | 79 | | TYR A | 12 | | 39.869 | 39.560 | 52.476 | 1.00 36.18 | 6 |
| ATOM | | | TYR A | 12 | | 39.533 | 39.479 | 49.721 | 1.00 37.69 | 6 |
| ATOM | 80 | | | | | 39.868 | 38.316 | 50.415 | 1.00 35.83 | 6 |
| ATOM | 81 | | TYR A | 12 | | | 38.365 | 51.787- | 1.00 34.10 | 6 |
| MOTA | 82 | CZ | TYR A | 12 | | 40.032 | | 52.470 | 1.00 36.31 | 8 |
| ATOM | 83 | OH | TYR A | 12 | | 40.339 | 37.216 | | | 6 |
| ATOM | 84 | С | TYR A | 12 | | 38.786 | 42.966 | 47.378 | 1.00 46.56 | |
| | 85 | Ó | TYR A | 12 | | 37.821 | 42.476 | 46.791 | 1.00 47.38 | 8 |
| ATOM | | И | GLY A | 13 | | 39.138 | 44.247 | 47.278 | 1.00 47.28 | 7 |
| ATOM . | 86 | | | | | 38.385 | 45.164 | 46.442 | 1.00 46.53 | 6 |
| MOTA | 87 | CA | GLY A | 13 | | | 44.934 | 44.968 | 1.00 45.60 | 6 |
| MOTA | 88 | С | GLY A | 13 | | 38.650 | | 44.117 | 1.00 43.68 | 8 |
| ATOM | 89 | 0 | GLY A | 13 | | 37.895 | 45.401 | | | 7 |
| ATOM | 90 | N | LYS A | 14 | | 39.725 | 44.210 | 44.672 | 1.00 46.52 | |
| MOTA | 91 | CA | LYS A | 14 | | 40.112 | 43.908 | 43.296 | 1.00 47.28 | 6 |
| | 92 | CB | LYS A | 14 | | 41.629 | 43.748 | 43.201 | 1.00 50.22 | 6 |
| ATOM | | CG | LYS A | 14 | | 42.396 | 45.044 | 43.307 | 1.00 57.12 | 6 |
| ATOM | 93 | | | | | 42.038 | 46.004 | 42.161 | 1.00 63.60 | 6 |
| ATOM | 94 | CD | LYS A | 14 | | 42.349 | 45.422 | 40.768 | 1.00 66.65 | 6 |
| ATOM | 95 | CE | LYS A | 14 | | | | 40.387 | 1.00 67.70 | 7 |
| - MOTA | 96 | NZ | LYS A | 14 | | 41.529 | 44.220 | 42.769 | 1.00 44.18 | 6 |
| MOTA | 97 | С | LYS A | 14 | | 39.460 | 42.643 | | 1.00 40.33 | 8 |
| MOTA | 98 | 0 | LYS A | 14 | | 39.564 | 42.325 | 41.585 | | 7 |
| ATOM | 99 | N | TYR A | 15 | | 38.790 | 41.926 | 43.661 | 1.00 43.25 | |
| | 100 | CA | TYR A | 15 | | 38.145 | 40.665 | 43.317 | 1.00 43.18 | 6 |
| ATOM | 101 | CB | TYR A | 15 | | 38.789 | 39.547 | 44.142 | 1.00 36.88 | 6 |
| MOTA | | | TYR A | 15 | | 40.302 | 39.560 | 44.053 | 1.00 32.96 | 6 |
| ATOM | 102 | CG | | | | 41.084 | 39.107 | 45.108 | 1.00 30.90 | 6 |
| MOTA | 103 | CD1 | TYR A | 15 | | 42.476 | 39.144 | 45.035 | 1.00 30.94 | 6 |
| MOTA | 104 | CE1 | TYR A | 15 | | | 40.049 | 42.912 | 1.00 33.01 | 6 |
| ATOM | 105 | CD2 | TYR A | 15 | | 40.952 | 40.092 | 42.826 | 1.00 29.68 | 6 |
| MOTA | 106 | CE2 | TYR A | 15 | | 42.341 | | | 1.00 30.99 | 6 |
| ATOM | 107 | CZ | TYR A | 15 | | 43.098 | 39.639 | 43.890 | | 8 |
| ATOM | 108 | OH | TYR A | 15 | | 44.471 | 39.673 | 43.809 | 1.00 28.02 | 6 |
| ATOM | 109 | С | TYR A | 15 | | 36.661 | 40.778 | 43.621 | 1.00 45.56 | |
| | 110 | ō | TYR A | 15 | | 36.149 | 40.153 | 44.552 | 1.00 45.22 | 8 |
| ATOM | 111 | N | ARG A | 16 | | 35.981 | 41.599 | 42.830 | 1.00 48.81 | 7 |
| ATOM | | | | 16 | | 34.553 | 41.819 | 42.999 | 1.90 53.22 | 6 |
| MOTA | 112 | CA | ARG A | | | 34.193 | 43.263 | 42.654 | 1 JO 57.11 | 5 |
| MOTA | 113 | CB | ARG A | 16 | | 34.852 | 44.330 | 43.490 | ·1 10 61.66 | 6 |
| ATOM | 114 | CG | ARG A | 16 | | | 44.408 | 44.886 | 1.00 67.04 | 6 |
| ATOM | 115 | CD | ARG A | 16 | | 34.280 | | 45.569 | 1.00 73.59 | 7 |
| ATOM | 116 | NE | ARG A | 16 | | 34.798 | 45.590 | | 1.00 75.03 | 6 |
| ATOM | 117 | CZ | ARG A | 16 | | 34.612 | 46.837 | 45.141 | | 7 |
| ATOM | 118 | ·-NH1 | ARG A | 16 | | 33.917 | 47.065 | 44.033 | 1.00 73.03 | |
| | 119 | | ARG A | 16 | | 35.142 | 47.856 | 45.808 | 1.00 75.79 | 7 |
| ATOM | | | | | | 33.757 | 40.903 | 42.080 | 1.00 51.79 | 6 |
| MOTA | 120 | C | ARG A | | | 34.192 | 40.593 | 40.970 | 1.00 50.89 | 8 |
| MOTA | 121 | 0 | ARG A | | | 32.596 | 40.463 | 42.552 | 1.00 50.19 | 7 |
| ATOM | 122 | N | TYR A | | | | | 41.733 | 1.00 49.60 | 6 |
| ATOM | 123 | CA | TYR A | | | 31.737 | 39.634 | 42.528 | 1.00 45.80 | 6 |
| ATOM | 124 | CB | TYR A | 17 | | 30.534 | 39.119 | | | 6 |
| ATOM | 125 | CG | TYR A | 17 | | 30.803 | | 43.365 | | 6 |
| | 126 | | TYR A | | | 31.589 | 37.932 | 44.438 | | |
| ATOM | | CEI | TYR A | 17 | | 31.960 | 36.780 | 45.193 | 1.00 43.36 | 6 |
| ATOM | 127 | | | | | 30.185 | | 43.062 | | 6 |
| ATOM | 128 | CD2 | TYR A | | | 30.443 | | 43.803 | | 6 |
| ATOM | 129 | CE2 | TYR A | | | | | | | 6 |
| ATOM | 130 | CZ | TYR A | | | 31.333 | | 45 | | 8 |
| ATOM | 131 | OH | TYR A | | | 31.600 | | 40 | | 6 |
| ATOM | 132 | С | TYR A | . 17 | | 31.245 | 40.547 | 40.622 | 1.00 31.00 | - |
| 71.01. | | | | ٠. | • | | | | | |
| • | | | | • | | | | | | |

| ATOM | 133 | 0 | TYR A | 1 17 | | 31.332 | 41.772 | 40.726 | 1.00 47.86 | 8 |
|--------|-----|-----|---------|------|----|--------|--------|--------|--------------|-----|
| ATOM | 134 | | PRO A | | | 30.730 | 39.964 | 39.534 | 1.00 54.38 | 7 |
| ATOM | 135 | | | | | 30.548 | 38.545 | | | |
| | | | | | | | | 39.190 | 1.00 54.21 | 6 |
| ATOM | 136 | | | | | 30.243 | 40.809 | 38.449 | 1.00 56.43 | 6 |
| ATOM | 137 | | | | | 29.601 | 39.792 | 37.496 | 1.00 56.84 | 6 |
| ATOM - | 138 | CG | PRO A | 18 | | 29.260 | 38.613 | 38.426 | 1.00 56.46 | 6 |
| MOTA | 139 | С | PRO A | 18 | | 29.273 | 41.891 | 38.932 | 1.00 58.74 | 6 |
| ATOM | 140 | 0 | PRO A | . 18 | | 28.791 | 41.861 | 40.066 | 1.00 55.72 | 8 |
| ATOM . | 141 | N | LYS A | | | 29.017 | 42.851 | 38.052 | 1.00 62.10 | 7 |
| ATOM | 142 | | LYS A | | | 28.127 | 43.973 | 38.314 | 1.00 64.85 | 6 |
| | | | | | | 27.972 | | | | |
| MOTA | 143 | | LYS A | | | | 44.781 | 37.022 | 1.00 69.74 | 6 |
| MOTA | 144 | | LYS A | | | 28.008 | 43.925 | 35.740 | 1.00 74.99 | 5 |
| ATOM | 145 | | LYS A | | - | 26.895 | 42.881 | 35.668 | - 1.00 78.18 | 6 |
| ATOM | 146 | CE | LYS A | 19 | | 26.981 | 42.010 | 34.420 | 1.00 80.24 | · 6 |
| MOTA | 147 | NZ | LYS A | . 19 | | 25.867 | 41.010 | 34.361 | 1.00 81.13 | 7 |
| ATOM | 148 | С | LYS. A | 19 | | 26.750 | 43.619 | 38.869 | 1.00 64.77 | 6. |
| ATOM | 149 | 0 | LYS A | | | 26.414 | 43.961 | 40.001 | 1.00 66.50 | 8 |
| ATOM | 150 | N | ASN A | | | 25.957 | 42.933 | 38.062 | 1.00 63.75 | 7 |
| ATOM | 151 | CA | ASN A | | | 24.612 | 42.556 | 38.439 | | |
| | | | | | | | | | 1.00 62.96 | 6 |
| ATOM | 152 | CB | ASN A | | | 23.870 | 42.031 | 37.208 | 1.00 67.42 | 6 |
| ATOM | 153 | CG | ASN A | | | 22.392 | 41.833 | 37.459 | 1.00 72.29 | 6 |
| ATOM | 154 | | l asn a | | | 21.666 | 42.785 | 37.772 | 1.00 75.25 | . 8 |
| ATOM | 155 | ND: | 2 asn a | . 20 | | 21.931 | 40.594 | 37.322 | 1.00 74.38 | 7 |
| ATOM | 156 | С | ASN A | 20 | | 24.602 | 41.512 | 39.547 | 1.00 61.30 | 6 |
| ATOM | 157 | 0 | ASN A | 20 | | 23.629 | 40.773 | 39.698 | 1.00 61.49 | 8 |
| MOTA | 158 | N | HIS A | | | 25.681 | 41.444 | 40.321 | 1.00 57.30 | 7 |
| ATOM | 159 | CA | HIS A | | | 25.755 | 40.480 | 41.418 | 1.00 54.68 | 6 |
| MOTA | 160 | CB | HIS A | | | 27.071 | 39.700 | 41.373 | 1.00 52.63 | 6 |
| ATOM | 161 | CG | HIS A | | | 27.058 | 38.449 | 42.195 | 1.00 49.39 | |
| ATOM | 162 | | HIS A | | | 27.336 | 38.236 | | | 6 |
| | | | | | | | | 43.503 | 1.00 49.39 | 6 |
| ATOM | 163 | | HIS A | 21 | | 26.664 | 37.229 | 41.686 | 1.00 48.27 | 7 |
| ATOM | 164 | | HIS A | 21 | | 26.704 | 36.320 | 42.643 | 1.00 48.16 | 6 |
| ATOM | 165 | | HIS A | 21 | | 27.108 | 36.905 | 43.757 | 1.00 47.33 | 7 |
| MOTA | 166 | С | HIS A | 21 | | 25.664 | 41.215 | 42.760 | 1.00 52.89 | 6 |
| MOTA | 167 | 0 | HIS A | 21 | | 26.295 | 42.256 | 42.947 | 1.00 52.52 | 8 |
| ATOM | 168 | N | PRO A | 22 | | 24.880 | 40.679 | 43.713 | 1.00 50.81 | 7 |
| MOTA | 169 | CD | PRO A | 22 | | 24.076 | 39.444 | 43.661 | 1.00 48.50 | 6 |
| ATOM | 170 | CA | PRO A | 22 | | 24.734 | 41.310 | 45.029 | 1.00 48.02 | 6 |
| ATOM | 171 | CB | PRO A | 22 | | 23.860 | 40.308 | 45.783 | 1.00 47.45 | 6 |
| ATOM | 172 | CG | PRO A | .22 | | 22.990 | 39.754 | 44.667 | 1.00 47.76 | 6 |
| MOTA | 173 | c | PRO A | 22 | | 26.074 | 41.558 | 45.727 | 1.00 46.48 | 6 |
| ATOM | 174 | ō | PRO A | 22 | | 26.164 | 42.405 | | | 8 |
| | | | | | | | | 46.615 | 1.00 45.69 | 7 |
| ATOM | 175 | N | LEU A | 23 | | 27.107 | 40.816 | 45.318 | 1.00 44.97 | |
| ATOM | 176 | CA | LEU A | 23 | | 28.441 | 40.949 | 45.906 | 1.00 41.31 | 6 |
| ATOM | 177 | CB | LEU A | 23 | | 29.076 | 39.569 | 46.131 | 1.00 39.22 | 6 |
| ATOM | 178 | CG | LEU A | 23 | | 28.264 | 38.561 | 46.953 | 1.00 37.71 | 6 |
| ATOM | 179 | CD7 | LEŲ A | 23 | | 29.075 | 37.288 | 47.157 | 1.00 35.07 | 6 |
| ATOM | 180 | CD2 | LEU A | 23 | | 27.896 | 39.165 | 48.292 | 1.00 36.90 | 6 |
| MOTA | 181 | С | LEU A | 23 | | 29.334 | 41.789 | 45.003 | 1.00 40.14 | 6 |
| ATOM | 182 | 0 | LEU A | 23 | | 30.556 | 41.614 | 44.951 | 1.00 39.00 | 8 |
| ATOM | 183 | N | LYS A | 24 | | 28.706 | 42.705 | 44.284 | 1.00 39.67 | 7 |
| ATOM | 184 | CA | LYS A | 24 | | 29.430 | 43.590 | | 1.00 42.88 | 6 |
| ATOM | 185 | СВ | LYS A | 24 | | 28.480 | 44.120 | 42.323 | 1.00 40.24 | 6 |
| | 186 | CG | LYS A | 24 | | 28.949 | 45.362 | 41.610 | 1.00 44.08 | 6 |
| ATOM | | | | | | | | | | |
| ATOM | 187 | CD | LYS A | 24 | | 28.247 | 46.600 | 42.166 | 1.00 44.47 | 6 |
| ATOM | 188 | CE | LYS A | 24 | | 26.732 | 46.492 | 41.968 | 1.00 43.23 | 6 |
| ATOM | 189 | NZ | LYS A | 24 | | 25.989 | 47.717 | 42.362 | 1.00 39.79 | 7 |
| ATOM | 190 | С | LYS A | 24 | | 30.031 | 44.723 | 44.217 | 1.00 43.70 | 6 |
| ATOM | 191 | 0 | LYS A | 24 | | 31.027 | 45.332 | 43.817 | 1.00 47.22 | 8 |
| ATOM | 192 | N | ILE A | 25 | | 29.431 | 44.976 | 45.378 | 1.00 42.27 | 7 |
| ATCM | 193 | CA | ILE A | 25 | | 29.870 | 46.035 | 46.289 | 1.00 39.86 | 6 |
| ATOM | 194 | CB | ILE A | 25 | | 28.763 | 46.407 | 47.306 | 1.00 37.72 | 6 |
| ATOM | 195 | CG2 | ILE A | 25 | | 27.539 | 46.953 | 46.580 | 1.00 39.67 | 6 |
| | | | | 25 | | 28.410 | | 48.145 | 1.00 35.25 | 6 |
| ATCM | 196 | | ILE A | | ٠. | 27.301 | 45.168 | 49.151 | 1.00 35.25 | 6 |
| ATOM | 197 | | ILE A | 25 | | | 45.368 | _ | 1.00 40.23 | 6 |
| ATCM | 198 | С | ILE A | . 25 | | 31.078 | 45.625 | 47.112 | 1.00 40.23 | 3 |
| | | • | - | | | | | | | |

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| | | | | | | | | | _ |
|---------|-------|------|-------|------|--------------------|--------|--------|--|-----|
| 3 0001/ | 199 | 0 | ILE A | 3 25 | 31.419 | 44.441 | 47.198 | 1.00 38.90 | 8 |
| MOTA | | | | | | 46.616 | 47.709 | 1.00 40.18 | 7 |
| ATOM | 200 | N | PRO A | A 26 | 31.762 | | | | |
| | 201 | CD | PRO A | A 26 | 31.523 | 48.051 | 47.533 | 1.00 40.58 | 6 |
| ATOM | | | | | 32,939 | 46.437 | 48.558 | 1.00 38.31 | 6 |
| ATOM | 202 | CA | PRO A | A 26 | | | | | |
| MOTA | 203 | CB | PRO A | A 26 | 33.478 | 47.860 | 48.688 | 1.00 37.14 | 6 |
| | | | | | 32.940 | 48.537 | 47.458 | 1.00 38.77 | 6 |
| ATOM | 204 | CG | PRO A | | | | | | 6 |
| ATOM | 205 | С | PRO A | A 26 | 32.433 | 45.903 | 49.891 | 1.00 37.32 | |
| | | Ō | PRO A | | 31.416 | 46.372 | 50.412 | 1.00 32.70 | 8 |
| MOTA | 206 | U | | | | | | 1.00 36.54 | 7 |
| ATOM | 207 | N . | ARG A | A 27 | 33.134 | 44.930 | 50.452 | and the second s | |
| | 208 | CA | ARG A | A 27 | 32.685 | 44.359 | 51.711 | 1.00 37.39 | 6 |
| MOTA | | | | | | 42.952 | 51.455 | 1.00 35.29 | 6 |
| MOTA | 209 | CB | ARG A | A 27 | | | | | |
| | 210 | CG | ARG A | A 27 | 31.047 | 42.956 | 50.355 | 1.00 32.69 | 6 |
| MOTA | | | | | 30.507 | 41.573 | 49.956 | 1.00 33.87 | 6 |
| ATOM | 211 | CD | ARG A | | | | | | 7 |
| MOTA | 212 | NE | ARG A | A 27 | 29.757 | 40.909 | 51.021 | 1.00 36.16 | |
| | | CZ | ARG A | A 27 | 30.293 | 40.132 | 51.959 | 1.00 37.11 | 6 |
| MOTA | 213 | | | | | | 51.976 | 1.00 34.42 | 7 |
| ATOM | 214 | NH1 | ARG A | A 27 | 31.604 | 39.903 | | | |
| | 215 | MH2 | ARG A | A 27 | 29.516 | 39.597 | 52.896 | 1.00 33.67 | 7 |
| ATOM | | | | | | 44.329 | 52.732 | 1.00 36.35 | 6 |
| MOTA | 216 | С | ARG A | | 33.813 | | | | |
| ATOM | 217 | 0 | ARG A | A 27 | 33.881 | 45.188 | 53.610 | 1.00 35.77 | 8 |
| | | | VAL A | | 34.703 | 43.351 | 52.607 | 1.00 34.93 | 7 |
| MOTA | 218 | N | | | | | 53.537 | 1.00 34.00 | 6 |
| ATOM | 219 | CA | VAL A | A 28 | 35.810 | 43.230 | | | |
| | 220 | CB | VAL A | A 28 | 36.633 | 41.954 | 53.252 | 1.00 36.21 | 6 |
| MOTA | | | | | 37.574 | 41.652 | 54.424 | 1.00 33.59 | 6 |
| ATOM | 221 | | VAL A | | | | | | 6 |
| ATOM | 222 | CG2 | VAL A | A 28 | 35.69 6 | 40.790 | 52.992 | 1.00 37.05 | |
| | 223 | C | VAL A | | 36.712 | 44.454 | 53.423 | 1.00 31.91 | 6 |
| ATOM | | | | | | 44.959 | 54.427 | 1.00 31.45 | 8 |
| ATOM | 224 | 0 | VAL A | A 28 | 37.216 | | | | 7 |
| ATOM | 225 | N | SER 2 | A 29 | 36.908 | 44.936 | 52.199 | 1.00 33.12 | |
| | 226 | CA | SER A | A 29 | 37.751 | 46.111 | 51.967 | 1.00 32.03 | 6 |
| ATOM | _ | | | - | | 46.181 | 50.499 | 1.00 31.77 | 6 |
| ATOM | 227 | CB . | SER I | | 38.205 | | | | 8 |
| MOTA | 228 | OG | SER : | A 29 | 37.113 | 46.223 | 49.600 | 1.00 30.80 | |
| | 229 | С | SER . | A 29 | 37.003 | 47.380 | 52.353 | 1.00 30.16 | 6 |
| MOTA | | | | | 37.604 | 48.404 | 52.650 | 1.00 28.70 | 8 |
| ATOM | 230 | 0 | SER . | A 29 | | | | 1.00 32.43 | 7 |
| MOTA | 231 | N | LEU . | A 30 | 35.682 | 47.310 | 52.352 | | |
| | 232 | CA | LEU . | | 34.900 | 48:465 | 52.745 | 1.00 34.56 | 6 |
| MOTA | | | | | 33.463 | 48.358 | 52.221 | 1.00 36.44 | б |
| MOTA . | 233 | CB | LEU . | | | | | 1.00 36.79 | 6 |
| MOTA | 234 | CG | LEU . | A 30 | 32.508 | 49.513 | 52.560 | | |
| | 235 | | LEU . | A 30 | 32.070 | 49.446 | 54.012 | 1.00 36.73 | 6 |
| ATOM | | | | | 33.202 | 50.840 | 52.256 | 1.00 37.84 | 6 |
| MOTA | 236 | CDZ | LEU . | | | | | 1.00 34.89 | 6 |
| MOTA | 237 | С | LEU . | A 30 | 34.902 | 48.527 | 54.262 | | |
| | 238 | 0 | LEU . | A 30 | 35.033 | 49.601 | 54.841 | 1.00 37.58 | 8 |
| MOTA | | | | | 34.761 | 47.366 | 54.897 | 1.00 34.07 | 7 |
| ATOM | 239 | N | LEU . | | | | 56.350 | 1.00 34.85 | 6 |
| ATOM | 240 | CA | LEU . | A 31 | 34.743 | 47.276 | | | |
| | 241 | CB | LEU . | A 31 | 34.768 | 45.808 | 56.791 | 1.00 36.37 | 6 |
| ATOM | | | | | 34.459 | 45.471 | 58.261 | 1.00 36.04 | 6 |
| MOTA | 242 | CG | LEU . | | | | | 1.00 35.13 | 6 |
| ATOM | 243 | CD1 | LEU . | A 31 | 34.841 | 44.027 | 58.532 | | |
| ATOM | 244 | CD2 | LEU . | A 31 | 35.228 | 46.357 | 59.194 | 1.00 35.86 | . 6 |
| | | | | | 35.976 | 47.994 | 56.894 | 1.00 36.43 | · 6 |
| MOTA | 245 | C | LEU . | | | 49.035 | 57.544 | 1.00 35.87 | 8 |
| ATOM | 246 | 0 | LEU | A 31 | 35.855 | | | | 7 |
| | 247 | N | LEU | A 32 | 37.157 | 47.426 | 56.635 | 1.00 37.76 | |
| ATOM | | | | | 38.420 | 48.015 | 57.087 | 1.00 36.82 | ő |
| ATCM | 248 | CA | LEU | | | 47.318 | 56.418 | 1.00 36.37 | 6 |
| ATOM | 249 | CB | LEU | A 32 | 39.611 | 47.310 | | | |
| ATOM | 250 | CG | LEU . | A 32 | 40.030 | 45.888 | 56.774 | 1.00 39.11 | 6 |
| | | | | | 41.117 | 45.420 | 55.815 | 1.00 35.16 | 6 |
| MOTA | 251 | | LEU | | | | 58.214 | 1.00 37.73 | 6 |
| ATOM | 252 | CD2 | LEU | A 32 | 40.538 | 45.830 | | 1.00 37.73 | |
| | 253 | С | LEU | A 32 | 38.500 | 49.513 | 56.780 | 1.00 34.84 | 6 |
| ATOM | | | | | 38.846 | 50.326 | 57.644 | 1.00 36.58 | 8 |
| ATOM | 254 | 0 | LEU | | | | | 1.00 31.37 | 7 |
| ATOM | 255 | N | ARG | A 33 | 38.184 | 49.877 | 55.545 | | |
| | 256 | CA | ARG | | 38.247 | 51.270 | 55.150 | 1.00 32.53 | 6 |
| ATOM | | | | | 37.927 | 51.398 | 53.662 | 1.00 31.52 | 6 |
| ATOM | 257 ' | CB. | ARG | A 33 | | | | 1.00 35.88 | 6 |
| ATCM | 258 | CG | ARG | A 33 | 38.481 | 52.652 | 53.042 | | ž |
| | | | ARG | | 38.107 | 52.752 | 51.581 | 1.00 43.44 | 6 |
| ATOM | 259 | CD | | | | 51.583 | 50.811 | 1.00 48.37 | 7 |
| ATCM | 260 | NE | ARG | | 38.521 | | | 1.00 52.27 | 6 |
| ATCM | 261 | CZ | ARG | A 33 | 38.348 | 51.469 | 49.497 | | |
| | | | ARG | | 37.771 | 52.459 | 48.823 | 1.00 51.75 | 7 |
| ATCM | 262 | MUT | MIG | ~ | | | 48.858 | 1.00 51.08 | 7 |
| atcm | 263 | NH2 | ARG | A 33 | 38.739 | 50.369 | | | 6 |
| ATCM | 264 | C | ARG | | 37.274 | 52.102 | 55.989 | 1.00 32.32 | 6 |
| | 203 | _ | | | | | - | | |



| MOTA | 265 | 0 | ·ARG | A 33 | 37.471 | 53.299 | 56.196 | 1.00 29.23 | 8 |
|--------------|------------|---------|------------|------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 266 | i N | PHE | A 34 | 36.231 | 51.445 | 56.484 | 1.00 32.58 | 7 |
| MOTA | 267 | 7 CA | PHE | A 34 | 35.216 | 52.096 | 57.304 | 1.00 32.69 | 6 |
| MOTA | 268 | CB | PHE | A 34 | 33.952 | 51.232 | 57.359 | 1.00 31.22 | 6 |
| MOTA | 269 | CG | PHE | A 34 | 32.838 | 51.825 | 58.183 | 1.00 28.74 | 6 |
| MOTA | 270 | | | | 32.085 | | 57.700 | 1.00 22.76 | 6 |
| MOTA | 271 | | | | 32.551 | | 59.456 | 1.00 28.09 | 6 |
| MOTA | 272 | | 1 PHE | | 31.061 | | 58.472 | 1.00 23.70 | 6 |
| MOTA | 273 | | | | 31.524 | | 60.235 | 1.00 24.59 | 6 |
| ATOM | 274 | | PHE | | 30.781 | | 59.741 | 1.00 21.39 | 6 |
| MOTA | 275 | | PHE | | 35.734 | | 58.719 | 1.00 33.45 | 6 |
| ATOM | 276 | | PHE | | 35.635 | | 59.258 | 1.00 35.49 | 8 |
| MOTA | 277 | | LYS | | 36.276 | | 59.323 | 1.00 34.52 | 7 |
| MOTA | 278 279 | | LYS | | 36.805 | | 60.678 | 1.00 36.51 | 6 |
| MOTA MOTA | 280 | | LYS LYS | | 37.118 35.912 | 49.977 49.074 | 61.235 | 1.00 36.47 | 6 |
| ATOM | 281 | | LYS | | 36.246 | | 61.343 | 1.00 40.81 | 6 |
| MOTA | 282 | | LYS | | 37.347 | 47.029 | 62.090 61.402 | 1.00 44.10 | 6 |
| ATOM | 283 | NZ | LYS | | 38.601 | 47.823 | 61.276 | 1.00 53.53 | 6 7 |
| ATOM | 284 | C | LYS | | 38.054 | 52.222 | 60.735 | 1.00 36.61 | 6 |
| ATOM | 285 | ō | LYS | | 38.352 | 52.824 | 61.766 | 1.00 36.78 | 8 |
| ATOM | 286 | N | ASP | | 38.794 | 52.267 | 59.635 | 1.00 36.27 | 7 |
| MOTA | 287 | CA | ASP | | 39.980 | 53.090 | 59.592 | 1.00 39.71 | 6 |
| ATOM | 288 | CB | ASP 2 | A 36 | 40.679 | 52.937 | 58.239 | 1.00 44.78 | 6 |
| MOTA | 289 | CG | | A 36 | 41.863 | 53.892 | 58.075 | 1.00 47.10 | 6 |
| ATOM | 290 | OD: | L ASP | A 36 | 42.803 | 53.852 | 58.906 | 1.00 44.02 | 8 |
| ATOM | 291 | | ASP A | A 36 | 41.843 | 54.682 | 57.106 | 1.00 48.43 | 8 |
| MOTA | 292 | C | ASP A | | 39.508 | 54.530 | 59.789 | 1.00 39.99 | 6 |
| MOTA | 293 | 0 | ASP Z | | 40.023 | 55.258 | 60.636 | 1.00 40.76 | 8 |
| MOTA | 294 | N | ALA A | | 38.506 | 54.919 | 59.007 | 1.00 38.59 | 7 |
| MOTA | 295 | CA | ALA A | | 37.939 | 56.258 | 59.066 | 1.00 37.14 | 6 |
| ATOM | 296 297 | CB C | ALA A | | 36.857 | 56.402 | 58.000 | 1.00 35.85 | 6 |
| ATOM ATOM | 298 | ò | ALA A | | 37.354 37.391 | 56.549 57.687 | 60.446 60.928 | 1.00 38.34 | 6 |
| ATOM | 299 | N | MET A | | 36.809 | 55.518 | 61.079 | 1.00 37.32 1.00 36.19 | 8 7 |
| ATOM | 300 | CA | MET A | | 36.213 | 55.674 | 62.397 | 1.00 36.80 | 6 |
| ATOM | 301 | CB | MET A | | 35.141 | 54.598 | 62.606 | 1.00 37.38 | 6 |
| ATOM | 302 | CG | MET A | | 33.938 | 54.717 | 61.673 | 1.00 37.60 | 6 |
| MOTA | 303 | SD | MET A | A 38 | 32.887 | 56.165 | 61.999 | 1.00 33.61 | 16 |
| ATOM | 304 | CE | MET A | 38 | 32.398 | 55.824 | 63.680 | 1.00 35.60 | 6 |
| MOTA | 305 | С | MET A | 38 | 37.262 | 55.582 | 63.502 | 1.00 35.84 | 6 |
| MOTA | 306 | 0 | MET A | | 36.937 | 55.688 | 64.692 | 1.00 34.89 | 8 |
| ATOM | 307 | N | ASN A | | 38.518 | 55.400 | 63.100 | 1.00 33.83 | 7 |
| ATOM | 308 | CA | ASN A | | 39.626 | 55.264 | 64.044 | 1.00 34.94 | 6 |
| ATOM | 309 | CB | ASN A | | 39.897 | 56.582 | 64.775 | 1.00 32.48 | 6 |
| ATOM | 310 | CG | ASN A | | 40.213 | 57.717 | 63.825 | 1.00 32.34 | 6 |
| ATOM ATOM | 311 312 | ND2 | ASN A | | 41.128 39.455 | 57.621 | 63.009 | 1.00 31.85 | 8. |
| ATOM | 313 | C | ASN A | | 39.253 | 58.800 54.183 | 63.924 65.045 | 1.00 30.92 | 7 6 |
| ATOM | 314 | ō | ASN A | | 39.403 | 54.357 | 66.260 | 1.00 36.60 | 8 |
| ATOM | 315 | N | LEU A | | 38.752 | 53.067 | 64.518 | 1.00 30.00 | 7 |
| ATOM | 316 | CA | LEU A | | 38.341 | 51.933 | 65.336 | 1.00 37.40 | 6 |
| ATOM | 317 | CB | LEU A | | 36.863 | 51.622 | 65.086 | 1.00 41.35 | 6 |
| | 318 | CG | LEU A | | 35.858 | 52.712 | 65.476 | 1.00 42.69 | 6 |
| ATOM | 319 | | LEU A | 40 | 34.448 | 52.261 | 65.111 | 1.00 45.05 | 6 |
| ATOM | 320 | | LEU A | | 35.951 | 52.989 | 66.966 | 1.00 39.44 | 6 |
| ATOM | 321 | С | LEU A | 40 | 39.184 | 50.687 | 65.058 | 1.00 39.79 | 6 |
| ATOM | 322 | 0 | LEU A | 40 | 38.804 | 49.575 | 65.434 | 1.00 36.88 | . 8 |
| ATOM | 323 | N | ILE A | 41 | 40.337 | 50.889 | 64.420 | 1.00 40.50 | 7 |
| ATOM | 324 | CA | ILE A | 41 | 41.237 | 49.790 | 64.068 | 1.00 41.39 | 6 |
| ATOM | 325 | CB | ILE A | 41 | 40.780 | 49.141 | 62.724 | 1.00 39.24 | 6 |
| MOTA | 326 | | ILE A | 41 | 41.017 | 50.103 | 61.564 | 1.00 36.97 | 6 |
| ATOM | 327 | | ILE A | 41 | 41.513 | 47.824 | 62.482 | 1.00 36.76 | 6 |
| MOTA | 328 | | ILE A | 41 | 41.085 | 46.715 | 63.403 | 1.00 35.59 | 6 |
| MOTA | 329 | c | ILE A | 41 | 42.684 | 50.295 | 63.913 | 1.00 44.37 | 6 |
| ATOM | 330 | 0 | ILE A | 41 | 42.927 | 51,328 | 63.277 | 1.00 46.01 | 8 |

| ATOM | 331 | N | ASP . | A 42 | 43.646 | 49.582 | 64.497 | 1.00 45.19 | 7 |
|--------|------|-----|-------|--------|----------|--------|--------|------------|----|
| | 332 | CA | ASP | | 45.049 | 49.982 | 64.372 | 1.00 45.62 | 6 |
| MOTA | | | | | | | | | |
| MOTA | 333 | CB | ASP . | A 42 | 45.716 | 50.090 | 65.742 | 1.00 45.17 | 6 |
| MOTA | 334 | CG | ASP . | A 42 | 44.966 | 51.005 | 66.682 | 1.00 44.43 | 6 |
| | 335 | | ASP . | | 44.731 | 52.177 | 66.322 | 1.00 39.84 | 8 |
| ATOM | | | | | | | | | |
| ATOM | 336 | OD2 | ASP . | A 42 | 44.612 | 50.546 | 67.787 | 1.00 48.50 | 8 |
| ATOM | 337 | С | ASP . | A 42 | 45.750 | 48.915 | 63.551 | 1.00 48.47 | 6 |
| | 33B | 0 | ASP | | 45.316 | 47.757 | 63.547 | 1.00 49.85 | 8 |
| ATOM | | | | | | | | | |
| MOTA | 339 | N | GLU . | A . 43 | 46.830 | 49.288 | 62.864 | 1.00 49.24 | 7 |
| ATOM | 340 | CA | GLU . | A 43 | 47.553 | 48.325 | 62.028 | 1.00 50.79 | 6 |
| | 341 | CB | GLU | | . 48.820 | 48.956 | 61.431 | 1.00 49.90 | 6 |
| MOTA | | | | | | | | | |
| ATOM | 342 | CG | GLU . | A 43 | 48.544 | 50.029 | 60.378 | 1.00 57.20 | 6 |
| ATOM | 343 | CD | GLU . | A 43 | 49.808 | 50.537 | 59.690 | 1.00 59.56 | 6 |
| | 344 | OE1 | | | 50.517 | 49.721 | 59.061 | 1.00 65.05 | 8 |
| MOTA | | | | | | | | | |
| MOTA | 345 | QE2 | GLU . | | 50.095 | 51.750 | 59.772 | 1.00 57.82 | 8 |
| ATOM | 346 | С | GLU . | A 43 | 47.918 | 47.020 | 62.733 | 1.00 49.73 | 6 |
| ATOM | 347 | 0 | GLU . | A 43 | 47.813 | 45.943 | 62.149 | 1.00 49.18 | 8 |
| | | | | | • | 47.118 | 63.992 | 1.00 49.40 | 7 |
| ATOM | 348 | N | LYS . | | 48.324 | | | | |
| ATOM | 349 | CA | LYS . | A 44 | 48.730 | 45.949 | 64.762 | 1.00 49.09 | 6 |
| MOTA | 350 | CB | LYS . | A 44 | 49.317 | 46.418 | 66.093 | 1.00 52.46 | 6 |
| | | CG | LYS | | 50.448 | 47.421 | 65.899 | 1.00 55.75 | 6 |
| MOTA | 351 | | | | | | | | |
| MOTA | 352 | CD | LYS . | A 44 | 51.167 | 47.749 | 67.201 | 1.00 58.74 | 6 |
| ATOM | 353 | CE | LYS . | A 44 | 52.327 | 48.704 | 66.949 | 1.00 58.48 | 6 |
| ATOM | 354 | NZ | LYS . | A 44 | 53.122 | 48.968 | 68.176 | 1.00 58.95 | 7 |
| | | | | | 47.638 | 44.897 | 64.994 | 1.00 47.63 | 6 |
| MOTA | 355 | С | LYS . | | | | | | |
| ATOM | 356 | 0 | LYS . | A 44 | 47.932 | 43.738 | 65.290 | 1.00 45.13 | 8 |
| ATOM | 357 | N | GLU . | a 45 | 46.379 | 45.298 | 64.854 | 1.00 45.25 | 7 |
| | 358 | CA | GLU . | | .45.268 | 44.374 | 65.046 | 1.00 43.09 | 6 |
| ATOM | | | | | | | | 1.00 41.19 | |
| MOTA | 359 | CB | GLU . | | 44.024 | 45.143 | 65.514 | | 6 |
| ATOM- | 360 | CG | GLU . | A 45 | 44.192 | 45.859 | 66.844 | 1.00 36.83 | 6 |
| ATOM | 361 | CD | GLU, | | 43.003 | 46.741 | 67.204 | 1.00 38.92 | 6 |
| | | | | | 42.707 | 47.701 | 66.447 | 1.00 37.30 | 8 |
| MOTA | 362 | | GLU . | = | | | | | |
| ATOM | 363 | OE2 | GLU . | A 45 | 42.368 | 46.479 | 68.253 | 1.00 36.33 | 8 |
| ATOM | 364 | С | GLU . | A 45 | 44.969 | 43.660 | 63.726 | 1.00 43.04 | 6 |
| | | | | | 44.480 | 42.523 | 63.699 | 1.00 45.03 | 8 |
| . MOTA | 365. | 0 | .GLU | | | | | | 7 |
| ATOM | 366 | N | LEU . | A 46 | 45.282 | 44.341 | 62.632 | 1.00 40.29 | |
| ATOM | 367 | CA | LEU . | A 46 | 45.042 | 43.823 | 61.299 | 1.00 37.16 | 6 |
| ATOM | 368 | CB | LEU . | | 44.910 | 44.990 | 60.331 | 1.00 37.86 | 6 |
| | | | | | | | 58.845 | 1.00 39.22 | 6 |
| ATOM | 369 | CG | LEU . | | 44.822 | 44.658 | | | |
| MOTA | 370 | CD1 | LEU . | A 46 | 43.655 | 43.726 | 58.563 | 1.00 40.68 | 6 |
| ATOM | 371 | CD2 | LEU . | A 46 | 44.673 | 45.964 | 58.080 | 1.00 41.62 | 6 |
| | | | LEU . | | 46.090 | 42.860 | 60.774 | 1.00 36.54 | 6 |
| ATOM | 372 | C | | | | | | | 8 |
| MOTA | 373 | 0 | LEU . | A 46 | 47.275 | 43.192 | 60.698 | 1.00 39.86 | |
| MOTA | 374 | N | ILE . | a 47 | 45.646 | 41.662 | 60.406 | 1.00 33.49 | 7 |
| ATOM | 375 | CA | ILE . | A 47 | 46.540 | 40.657 | 59.844 | 1.00 30.51 | 6 |
| | | | ILE . | | 46.333 | 39.253 | 60.491 | 1.00 34.31 | 6 |
| ATOM | 376 | CB | | | | | | | |
| ATOM | 377 | CG2 | ILE . | ል 47 | 47.346 | 38.262 | 59.930 | 1.00 32.16 | 6 |
| MOTA | 378 | CG1 | ILE . | a 47 | 46.504 | 39.328 | 62.010 | 1.00 32.65 | 6 |
| | 379 | | ILE | | 47.858 | 39.846 | 62.448 | 1.00 38.97 | 6 |
| ATOM | | | | | | | 58.362 | 1.00 28.36 | 6 |
| MOTA | 380 | C | ILE . | | 46.196 | 40.570 | | | |
| ATOM | 381 | 0 | ILE . | a 47 | 45.037 | 40.342 | 58.003 | 1.60 26.11 | 8 |
| ATOM | 382 | N | LYS 2 | A 48 | 47.194 | 40.772 | 57.504 | 1.00 27.77 | 7 |
| | | | | _ | 46.985 | 40.713 | 56.056 | 1.00 25.80 | 6 |
| ATOM | 383 | CA | LYS A | | | | | | |
| MOTA | 384 | CB | LYS . | A 48 | 48.258 | 41.087 | | 1.00 23.91 | 6 |
| MOTA | 385 | CG | LYS . | A 48 | 48.056 | 41.273 | 53.811 | 1.00 24.90 | 6 |
| | | CD | LYS . | | 49.389 | 41.352 | 53.091 | 1.00 26.39 | 6 |
| ATOM | 386 | | | - | | | | 1.00 27.71 | 6 |
| ATOM | 387 | CE | LYS . | | 49.233 | 41.864 | 51.679 | | 5 |
| ATOM | 388 | NZ | LYS | A 48 | 48.774 | 43.275 | 51.696 | 1.00 32.59 | 7 |
| | 389 | С | LYS . | | 46.595 | 39.299 | 55.654 | 1.00 26.32 | 6 |
| MOTA | | | | | | 38.325 | 56.235 | 1.00 27.85 | 8 |
| ATOM | 390 | 0 | LYS . | | 47.072 | | | | 7 |
| ATOM | 391 | N | SER . | A 49 | 45.735 | 39.183 | 54.653 | 1.00 24.73 | ′_ |
| ATOM | 392 | CA | SER . | | 45.299 | 37.876 | 54.205 | 1.00 27.36 | 6 |
| | | | SER . | | 43.952 | 37.979 | 53.479 | 1.00 25.04 | 6 |
| ATOM | 393 | CB | | | | | | 1.00 26.94 | 8 |
| MOTA | 394 | OG | SER . | | 42.911 | 38.329 | 54.373 | | |
| ATOM | 395 | С | SER : | A 49 | 46.322 | 37.211 | 53.293 | 1.00 28.97 | 6 |
| | 396 | ō | SER | | 47.095 | 37.885 | 52.612 | 1.00 31.89 | 8 |
| atom | 270 | v | | | , | | • | • | |
| • | | | - | | | | • | | |
| | | | | | | | | | |

| ATOM | 397 N ARG A 50 | 46.315 35.8 | 70 53 306 | | |
|--------|--------------------------------------|--------------------------------|------------------|--------------------------|-----|
| ATOM | 398 CA ARG A 50 | 47.211 35.0 | | | 7 |
| ATOM | 399 CB ARG A 50 | | | | 6 |
| ATOM | 400 CG ARG A 50 | | | | 6 |
| ATOM | 401 CD ARG A 50 | = | | | 6 |
| ATOM_ | 402 NE ARG A 50 | | | | 6 |
| ATOM | 403 CZ ARG A 50 | :: | | | · 7 |
| ATOM | 404 NH1 ARG A 50 | 47.708 30.30 | | 1.00 16.85 | 6 |
| MOTA | 405 NH2 ARG A 50 | 47.430 30.19 | 54.055 | 1.00 17.77 | 7 |
| MOTA | 406 C ARG A 50 | 47.334 29.31 | 56.223 | 1.00 14.56 | 7 |
| ATOM | 407 O ARG A 50 | 46.370 34.09 | _ | 1.00 23.30 | 6 |
| ATOM | 408 N PRO A 51 | 45.319 33.63 | | 1.00 16.92 | 8 |
| ATOM | 409 CD PRO A 51 | 46.823 33.62 | | 1.00 21.06 | 7 |
| ATOM | 410 CA PRO A 51 | 48.021 34.03 | | | 6 |
| ATOM | 444 | 46.086 32.63 | | 1.00 22.69 | 6 |
| ATOM | | 46.862 32.59 | | 1.00 21.57 | 6 |
| ATOM | 444 | 47.503 33.98 | | 1.00 20.57 | 6 |
| ATOM | 4.4 | 46.153 31.30 | | 1.00 26.71 | 6 |
| ATOM | 44.5 | 47.071 31.06 | | 1.00 31.32 | 8 |
| ATOM | | 45.176 30.43 | | 1.00 26.02 | 7 |
| ATOM | 415 | 45.151 29.12 | | 1.00 25.76 | 6 |
| ATOM | | 43.720 28.58 | | 1.00 21.42 | 6 |
| ATOM | ****** | 46.013 28.22 | | 1.00 26.31 | 6 |
| ATOM | | .5.0,0 20.23 | | 1.00 30.31 | . 8 |
| ATOM | 404 | 46.909 27.46 | | 1.00 26.80 | 7 |
| ATOM | | 47.759 26.57 | | 1.00 27.52 | 6 |
| ATOM | 400 | 48.845 25.97 | | 1.00 26.27 | 6 |
| ATOM | 101 | 48.255 25.05 | | 1.00 29.51 | 8 |
| ATOM | 424 CG2 THR A 53 425 C THR A 53 | 49.522 27.07 | | 1.00 24.66 | 6 |
| MOTA | 426 O THR A 53 | 46.908 25.46 | | 1.00 26.58 | 6 |
| ATOM | 427 N LYS A 54 | 45.778 25.22 | | 1.00 21.98 | 8 |
| ATOM | 428 CA LYS A 54 | 47.455 24.78 46.739 23.71 | – – – | 1.00 29.62 | 7 |
| ATOM | 429 CB LYS A 54 | | | 1.00 32.62 | 6 |
| ATOM | 430 00 110 5 | 47.601 23.15 | | 1.00 31.99 | 6 |
| ATOM | 430 CG LYS A 54 . 431 CD LYS A 54 | 46.985 21.96 45.733 22.35 | | 1.00 36.62 | 6 |
| ATOM | 432 CE LYS A 54 | | 44.866 | 1.00 40.69 | 6 |
| ATOM | 433 NZ LYS A 54 | 46.058 23.17 46.844 22.39 | | 1.00 46.44 | 6 |
| MOTA | 434 C LYS A 54 | | | 1.00 50.68 | 7 |
| ATOM | 435 O LYS A 54 | | | 1.00 36.00 | б |
| ATOM | 436 N GLU A 55 | 45.277 21.993 47.216 22.330 | | 1.00 34.77 | 8 |
| MOTA | 437 CA GLU A 55 | 46.979 21.29 | | 1.00 37.91 | 7 |
| ATOM | 438 CB GLU A 55 | 48.240 21.100 | | 1.00 36.96 | 6 |
| ATOM | 439 CG GLU A 55 | 48.216 19.887 | | 1.00 40.29 | 6 |
| ATOM | 440 CD GLU A 55 | 49.552 19.654 | | 1.00 47.95 | 6 |
| ATOM | 441 OE1 GLU A 55 | 49.659 18.688 | | 1.00 51.01 | 6 |
| MOTA | 442 OE2 GLU A 55 | 50,497 20.437 | | 1.00 52.65 | 8 |
| ATOM | 443 C GLU A 55 | 45.771 21.609 | | 1.00 51.27 | 8 |
| ATOM - | 444 O GLU A 55 | 44.892 20.769 | | 1.00 34.10 | 6 |
| ATOM | 445 N GLUA 56 | 45.723 22.827 | | 1.00 33.08 1.00 32.39 | 8 |
| ATOM | 446 CA GLU A 56 | 44.621 23.256 | | 1.00 32.39 | 7 |
| ATOM | 447 CB.GLU A 56 | 44.824 24.714 | 53.177 | 1.00 30.13 | 6 |
| ATOM | 448 CG GLU A 56 | 46.204 24.994 | 53.758 | 1.00 28.82 | 6 |
| ATOM | 449 CD GLU A 56 | 46.421 26.450 | 54.181 | 1.00 28.82 | 6 |
| MOTA | 450 OE1 GLU A 56 | 46.072 27.369 | 53.398 | 1.00 30.74 | 6 |
| ATOM | 451 OE2 GLU A 56 | 46.969 26.674 | 55.288 | 1.00 29.77 | 8 |
| MOTA | 452 C GLU A 56 | 43.264 23.114 | 52.024 | 1.00 25.98 | 8 |
| ATOM | 453 O GLU A 56 | 42.299 22.584 | 52.595 | 1.00 29.63 | 6 |
| atom | 454 N LEU A 57 | 43.188 23.581 | | 1.00 29.90 | 8 |
| ATOM | 455 CA LEU A 57 | 41.944 23.490 | 50.780 | 1.00 26.76 | 7 |
| ATOM | 456 CB LEU A 57 | 42.132 24.103 | 50.020 | 1.00 25.29 | 6 |
| ATOM | 457 CG LEU A 57 | 42.402 25.612 | 48.629 48.572 | 1.00 22.68 | 6 |
| ATOM | 458 CD1 LEU A . 57 | 42.654 26.045 | 48.572 | 1.00 22.39 | 5 |
| ATOM | 459 CD2 LEU A 57 | 41.211 26.366 | 49.156 | 1.00 20.77 | 6 |
| ATOM | 460 C LEU A 57 | 41.479 22.037 | | 1.00 17.66 | 6 |
| | .461 O LEU A 57 | 40.284 21.741 | | 1.00 26.02 1.00 23.41 | 6 |
| ATOM | 462 N LEU A 58 | 42.444 21.143 | 49.675 | 1.00 23.41 | 8 |
| | | 21.143 | 43.0/J | 1.00 24.82 | 7 |
| | | | | | |

| ATOM | 463 | CA | LEU | Α . | 58 | 42 | 2.194 | 19.718 | 49.526 | 1.00 | 22.44 | 6 |
|------------------|-----|-----|-----|-----|----------|-----|-------|--------|--------|------|-------|-----|
| | | | | | 58 | | 3.434 | 19,027 | 48.965 | 1.00 | 21 02 | 6 |
| ATOM | 464 | СВ | LEU | | | | | | | | | |
| MOTA | 465 | CG | LEU | A : | 58 | 43 | 3.838 | 19.471 | 47.558 | 1.00 | | 6 |
| ATOM | 466 | CD1 | LEU | A 1 | 58 | 45 | 5.212 | 18.908 | 47.176 | 1.00 | 20.35 | 6 |
| | | | | | 58 | | 2.755 | 19.033 | 46.587 | 1.00 | 23 28 | 6 |
| ATOM | 467 | | LEU | | | | | | | | | |
| MOTA | 468 | С | LEU | A : | 58 | 43 | 1.797 | 19.054 | 50.835 | | 25.20 | 6 |
| MOTA | 469 | 0 | LEU | Α ! | 38 | 43 | 1.456 | 17.867 | 50.854 | 1.00 | 26.55 | 8 |
| _ | | | | | 59 | | 1.858 | 19.794 | 51.938 | 1.00 | 25 44 | 7 |
| MOTA | 470 | N | LEU | | | | | | | | | |
| ATOM | 471 | CA | LEU | A : | 59 | 4. | 1.446 | 19.212 | 53.211 | 1.00 | | 6 |
| ATOM | 472 | CB | LEU | A ! | 59 | 41 | 1.559 | 20.229 | 54.350 | 1.00 | 24.68 | 6 |
| | | | | | 59 | | 2.956 | 20.490 | 54.912 | 1.00 | 27 05 | 6 |
| ATOM | 473 | CG | LEU | | | | | | | | | |
| MOTA | 474 | CD1 | LEU | A : | 59 | 42 | 2.912 | 21.565 | 56.001 | 1.00 | | 6 |
| MOTA | 475 | CD2 | LEU | A ! | 59 | 4: | 3.492 | 19.184 | 55.474 | 1.00 | 26.99 | 6 |
| | 476 | C | LEU | | 59 | 3 (| 9.991 | 18.807 | 53.045 | 1.00 | 24.22 | 6 |
| ••• | | | | | | | | | 53.581 | 1.00 | | 8 |
| ATOM | 477 | 0 | LEU | | 59 | | 9.548 | 17.794 | | | | |
| MOTA | 478 | N | PHE | A (| 60 | 3 | 9.270 | 19.615 | 52.270 | 1.00 | 25.00 | 7 |
| ATOM | 479 | CA | PHE | Δ , | 60 | 31 | 7.859 | 19.403 | 52.011 | 1.00 | 25.00 | 6 |
| | | | | | | | 7.054 | 20.560 | 52.605 | 1.00 | 26 34 | 6 |
| ATOM | 480 | CB | PHE | | 60 | | | | | | | |
| MOTA | 481 | CG | PHE | A (| 60 · | 3: | 5.600 | 20.555 | 52.223 | 1.00 | | 6 |
| MOTA | 482 | CD1 | PHE | A | 60 | 3 | 4.811 | 19.422 | 52.427 | 1.00 | 27.57 | 6 |
| | 483 | | PHE | | 60 | 31 | 5.015 | 21.692 | 51.661 | 1.00 | 27.33 | 6 |
| MOTA | | | | | | | | | 52.077 | 1.00 | | 6 |
| MOTA | 484 | | PHE | | 60 | | 3.466 | 19.419 | | | | |
| ATOM | 485 | CE2 | PHE | A | 60 | 3: | 3.670 | 21.699 | 51.306 | | 28.08 | 6 |
| ATOM | 486 | CZ | PHE | Α : | 60 | 3: | 2.893 | 20.559 | 51.513 | 1.00 | 29.48 | 6 |
| | | | | | 60 | | 7.506 | 19.214 | 50.538 | | 27.78 | 6 |
| ATOM | 487 | С | PHE | | | | | | | | | . 8 |
| ATOM | 488 | 0 | PHE | Α | 60 | | 7.022 | 18.143 | 50.158 | | 31.57 | |
| ATOM | 489 | N | HIS | A | 61 | 3' | 7.734 | 20.220 | 49.696 | 1.00 | 26.76 | 7 |
| | 490 | CA | HIS | | 61 | 3, | 7.376 | 20.056 | 48.287 | 1.00 | 28.84 | 6 |
| ATOM | | | | | | | 7.365 | 21.405 | 47.561 | | 27.76 | 6 |
| MOTA | 491 | CB | HIS | | 61 | | | | | | | 6 |
| MOTA | 492 | CG | HIS | A | 61 | 3 | 6.385 | 22.396 | 48.117 | | 30.54 | |
| ATOM | 493 | CD2 | HIS | A | 61 | 3: | 5.056 | 22.549 | 47.907 | 1.00 | 33.74 | 6 |
| | 494 | | HIS | | 61 | 3 | 6.750 | 23.401 | 48.987 | 1.00 | 34.02 | 7 |
| ATOM | | | | | | | 5.691 | 24.135 | 49.286 | 1.00 | 32.07 | 6 |
| MOTA | 495 | | HIS | | 61. | | | • | | | | 7 |
| MOTA | 496 | NE2 | HIS | A · | 61 | 3. | 4.649 | 23.638 | 48.644 | | 34.10 | |
| ATOM | 497 | С | HIS | A | 61 | 3 | 8.278 | 19.056 | 47.539 | 1.00 | 28.38 | 6 |
| | | | | | 61 | | 9.287 | 18.604 | 48.072 | 1.00 | 25.81 | 8 |
| MOTA | 498 | 0 | HIS | | | | | | | | 32.88 | 7 |
| ATOM | 499 | N | THR | A | 62 | | 7.895 | 18.705 | 46.310 | | | |
| ATOM | 500 | CA | THR | Α | 62 | 3. | 8.658 | 17.749 | 45.488 | | 34.68 | 6 |
| | 501 | CB | THR | Δ. | 62 | 3 | 7.715 | 16.739 | 44.778 | 1.00 | 34.36 | 6 |
| ATOM | | | | | 62 | | 6.942 | 17.415 | 43.778 | 1.00 | 34.81 | 8 |
| MOTA | 502 | | THR | | | | | | | | 34.33 | 6 |
| ATOM | 503 | CG2 | THR | A | 62 | 3 | 6.759 | 16.112 | 45.778 | 1.00 | | |
| ATOM | 504 | С | THR | A | 62 | 3: | 9.485 | 18.454 | 44.408 | 1.00 | 35.60 | 6 |
| | 505 | o | THR | | 62 | 3 | 9.017 | 19.418 | 43.790 | 1.00 | 30.85 | 8 |
| ATOM | | | | | | | 0.700 | 17.958 | 44.166 | 1.00 | 37.38 | 7 |
| MOTA | 506 | N | GLU | | 63 | | | | | | | 6 |
| MOTA | 507 | CA | GLU | A | 63 | 4 | 1.587 | 18.555 | 43.165 | | 40.68 | |
| ATOM | 508 | CB | GLU | Α | 63 | 4 | 2.759 | 17.626 | 42.840 | 1.00 | 43.75 | 6 |
| | 509 | CG | GLU | | 63 | | 3.719 | 17.389 | 43.987 | 1.00 | 50.68 | 6 |
| ATOM | | | | | | | | 16.760 | 43.529 | | 55.36 | 6 |
| ATOM | 510 | CD | GLU | | 63 | | 5.026 | | | | - | |
| ATOM | 511 | OE1 | GLU | A | 63 | 4 | 5.789 | 17.441 | 42.808 | 1.00 | 53.03 | 8 |
| MOTA | 512 | OE2 | GLU | Α | 63 | 4 | 5.285 | 15.585 | 43.883 | 1.00 | 59.56 | 8 |
| | | | | | 63 | | 0.894 | 18.939 | 41.860 | 1.00 | 39.26 | 6 |
| MOTA | 513 | C | GLU | | | _ | | | | | 42.33 | 8 |
| ATOM | 514 | 0 | GLU | | 63 | | 0.771 | 20.116 | 41.535 | | | |
| ATOM | 515 | N | ASP | A | 64 | 4 | 0.453 | 17.948 | 41.102 | | 37.07 | 7 |
| | 516 | CA | ASP | | 64 | 3 | 9.782 | 18.224 | 39.845 | 1.00 | 36.98 | 6 |
| MOTA | | | | | | | | 17.000 | 39.426 | | 42.19 | 6 |
| MOTA | 517 | CB | ASP | | 64 | | 8.957 | | | | _ | 6 |
| MOTA | 518 | CG | ASP | Α | 64 | 3 | 8.037 | 16.501 | 40.533 | | 47.66 | |
| ATOM | 519 | 001 | ASP | A | 64 | 3 | 7.039 | 17.193 | 40.851 | | 47.95 | 8 |
| | 520 | | ASP | | 64 | | 8.325 | 15.413 | 41.091 | 1.00 | 50.07 | .8 |
| MOTA | | | | | | | | | 39.906 | | 33.40 | 6 |
| MOTA | 521 | С | ASP | | 64 | | 8.908 | 19.480 | | | | |
| ATOM | 522 | 0 | ASP | А | 64 | 3 | 8.927 | 20.293 | 38.986 | | 33.64 | 8 |
| | 523 | N | TYR | | 65 | 3 | 8.156 | 19.641 | 40.990 | 1.00 | 30.57 | 7 |
| ATOM | | | | | | | 7.286 | 20.806 | 41.157 | | 29.65 | 6 |
| · ATOM | 524 | CA | TYR | | 65 55 | | | | 42.316 | 1.00 | _ | ő |
| MOTA | 525 | CB | TYR | | 65 | | 6.300 | 20.560 | | | | 6 |
| ATOM | 526 | CG | TYR | Α | 65 | 3 | 5.557 | 21.790 | 42.810 | | 28.49 | |
| | 527 | | TYR | | 65 | | 4.791 | 22.572 | 41.944 | 1.00 | 30.25 | 6. |
| ATOM | | | | | | | | 23.715 | 42.399 | | 28.36 | 6 |
| ATOM | 528 | - | TYR | A | 65 | ٠ 3 | 4.126 | 23.123 | | | 20.00 | |
| · - · | | | • • | | | | | | | • | | |
| | | | | | | | | | | | | |

| ATOM | 529 CD2 TYR A 65 | 35.638 22.181 44.150 1 00 28 28 6 |
|-------|-------------------------------------|--|
| ATOM | 530 CE2 TYR A 65 | 2. 1.00 28.28 6 |
| ATOM | 531 CZ TYR A 65 | 74 22 20,50 |
| ATOM | 532 OH TYR A 65 | 33.740 1.00 29.79 6 |
| MOTA | 533 C TYR A 65 | 38 119 22 061 41 41 |
| MOTA | 534 O TYR A 65 | 30 000 23.13 |
| ATOM | 535 N ILE A 66 | 30 100 20 30 30 |
| ATOM | 536 CA ILE A 66 | 70 006 17 |
| ATOM | 537 CB ILE A 66 | 40 200 20,33 6 |
| ATOM | 538 CG2 ILE A 66 | 40 000 00 00 00 00 00 00 00 00 00 00 00 |
| MOTA | 539 CG1 ILE A 66 | 42.009 23./53 43.869 1.00 21.20 6 |
| ATOM | 540 CD1 ILE A 66 | 40.264 22.341 44.992 1.00 29.30 6 |
| ATOM | 541 C ILE A 66 | 39.478 23.517 45.555 1.00 30.52 6 |
| ATOM | 542 O ILE A 66 | 40.761 23.504 41.381 1.00 28.07 6 |
| ATOM | 543 N ASN A 67 | 41.039 24.696 41.225 1.00 31.26 8 |
| ATOM | 544 CA ASN A 67 | 41.125 22.559 40.521 1.00 28.47 7 |
| ATOM | F 4 F | 41.902 22.898 39.337 1.00 30.15 6 |
| ATOM | 545 CB ASN A 67 546 CG ASN A 67 | 42.563 21.656 38.726 1.00 34.20 6 |
| ATOM | 547 OD1 ASN A 67 | 43.712 21.118 39.578 1.00 38.78 6 |
| ATOM | 548 ND2 ASN A 67 | 44.674 21.841 39.878 1.00 43.34 8 |
| ATOM | F 40 | 43.626 19.845 39.956 1.00 37.14 7 |
| MOTA | 550 - | 41.020 23.554 38.314 1.00 28.41 6 |
| ATOM | | 41.494 24.354 37.499 1.00 28.05 8 |
| ATOM | 550 | 39.733 23.221 38.361 1.00 25.32 7 |
| ATOM | rra | 38.787 23.791 37.416 1.00 21.75 6 |
| ATOM | 553 CB THR A 68 554 OG1 THR A 68 | 37.438 23.111 37.500 1.00 16.99 6 |
| ATOM | 555 CG2 THR A 68 | 37.020 21.695 37.371 1.00 16.99 8 |
| ATOM | 556 C THR A 68 | 36.549 23.591 36.359 1.00 17.59 6 |
| ATOM | 557 O THR A 68 | 38.633 25.263 37.732 1.00 22.13 6 |
| ATOM | 558 N LEU A 69 | 30.329 26.088 36.830 1 nn 21 a7 a |
| ATOM | 559 CA LEU A 69 | 38.645 25.582 39.023 1.00 22.32 7 |
| ATOM | 560 CB LEU A 69 | 38.535 26.956 39.482 1.00 23.97 6 |
| MOTA | 561 CG LEU A 69 | 38.376 26.982 41.000 1.00 24.99 6 |
| MOTA | 562 CD1 LEU A 69 | 37.023 26.527 41.548 1.00 29.08 6 |
| ATOM | 563 CD2 LEU A 69 | 37.087 26.416 43.066 1.00 30.99 6 |
| ATOM | 564 C LEU A 69 | 35.942 27.528 41.120 1.00 28.69 6 |
| ATOM | 565 O LEU A 69 | 39.772 27.757 39.088 1.00 24.90 6 |
| ATOM | 566 N MET A 70 | 39.683 28.921 38.674 1.00 25.04 8 |
| MOTA | 567 CA MET A 70 | 40.932 27.128 39.218 1.00 24.67 7 42.183 27.794 38.897 1.00 23.62 |
| ATOM | 568 CB MET A 70 | 13 22 0 |
| MOTA | 569 CG MET A 70 | 43 419 26 751 40 000 1.00 20.52 6 |
| ATOM | 570 SD MET A 70 | 44 000 |
| MOTA | 571 CE MET A 70 | 46 137 11.525 1.00 30.71 16 |
| ATOM | 572 C MET A 70 | 100 23.20 |
| ATOM | 573 O MET A 70 | 42 202 |
| ATOM | 574 N GLU A 71 | 41 760 27 122 26 622 |
| ATOM | 575 CA GLU A 71 | 41 000 00 00 |
| ATOM | 576 CB GLU A 71 | 1.00 24.41 |
| ATOM | 577 CG GLU A 71 | 3. 302 1.00 26.22 6 |
| MOTA | 578 CD GLU A 71 | 1.00 31.73 |
| ATOM. | 579 OE1 GLU A 71 | 1.00 33.00 6 |
| ATOM | 580 OE2 GLU A 71 | |
| ATOM | 581 C GLU A 71 | 1.00 30.13 |
| ATOM | 582 O GLUA 71 | 1.00 21.60 |
| ATOM | 583 N ALA A 72 | 20 21.34 8 |
| ATOM | 584 CA ALA A 72 | 30 500 |
| ATOM | 585 CB ALA A 72 | 37 300 30 500 35 |
| MOTA | 586 C ALA A 72 | 1.00 13.23 |
| MOTA | 587 O ALA A 72 | 20 700 20.72 |
| MOTA | 588 N GLU A 73 | |
| ATOM | 589 CA GLU A 73 | 1.00 20,44 |
| MOTA | 590 CB GLU A 73 | |
| MOTA | 591 CG GLU A 73 | 100 23.04 |
| ATOM | 592 CD GLU A 73 | 1.00 27.31 |
| ATOM | 593 OE1 GLU A 73 | 2.00 23.36 |
| ATOM | 594 OE2 GLU A 73 | |
| | | 41.996 33.960 40.277 1.00 31.77 8 |

| ATOM | 595 | С | GLU A | 73 | | 40.946 | 32.840 | 35.615 | 1.00 3 | 1.83 | 6 |
|--------|-------|----|--------|------|---|--------|--------|--------|--------|-------|----|
| MOTA | 596 | ō | GLU A | | | 40.859 | 34.024 | 35.259 | 1.00 3 | 3.52 | 8 |
| | 597 | N | ARG A | | | 41.992 | 32.071 | 35.309 | 1.00 3 | | 7 |
| MOTA | | | | | | 43.128 | 32.611 | 34.557 | 1.00 3 | | 6 |
| ATOM | 598 | CA | ARG A | | | | | | 1.00 3 | | 6 |
| MOTA | 599 | CB | ARG A | | | 44.405 | 31.826 | 34.874 | | | |
| ATOM | 600 | CG | ARG A | | | 44.514 | 30.467 | 34.205 | 1.00 3 | | 6 |
| MOTA | 601 | CD | ARG A | 74 | | 45.702 | 29.714 | 34.754 | 1.00 3 | | 6 |
| MOTA | 602 | NE | ARG A | 74 | • | 46.041 | 28.561 | 33.933 | 1.00 3 | 4.18 | 7 |
| ATOM | 603 | CZ | ARG A | 74 | | 46.646 | 28.634 | 32.748 | 1.00 3 | 5.55 | 6 |
| ATOM | 604 | | ARG A | | | 46.989 | 29.818 | 32.232 | 1.00 2 | 9.64 | 7 |
| MOTA | 605 | | ARG A | _ | _ | 46.906 | 27.514 | 32.079 | 1.00 3 | 4.07 | 7 |
| | 606 | C | ARG A | | | 42.894 | | 33.051 | 1.00 2 | | 6 |
| ATOM | | | | | | 43.431 | 33.465 | 32.338 | 1.00 2 | | 8 |
| ATOM . | 607 | 0 | ARG A | | | | 31.673 | 32.566 | 1.00 2 | | 7 |
| MOTA | 608 | N | CYS A | | | 42.107 | | | | | 6 |
| ATOM | 609 | CA | CYS A | | | 41.796 | 31.619 | 31.148 | 1.00 3 | | |
| MOTA | 610 | CB | CAR. Y | | | 41.687 | 30.167 | 30.682 | 1.00 3 | | 6 |
| MOTA | 611 | SG | CYS A | 75 | | 43.281 | 29.296 | 30.777 | 1.00 3 | | 16 |
| MOTA | 612 | C | CYS A | 75 | | 40.489 | 32.382 | 30.956 | 1.00 3 | | 6 |
| ATOM | 613 | 0 | CYS A | . 75 | • | 40.029 | 32.598 | 29.834 | 1.00 3 | 0.74 | 8 |
| ATOM | 614 | N | GLN A | . 76 | | 39.914 | 32.787 | 32.088 | 1.00 3 | 4.42 | 7 |
| ATOM | 615 | CA | GLN A | | | 38.691 | 33.575 | 32.144 | 1.00 3 | 3.20 | 6 |
| MOTA | 616 | CB | GLN A | | | 38.986 | 34.962 | 31.578 | 1.00 3 | 2.09 | 5 |
| | 617 | CG | GLN A | - | | 38.089 | 36.064 | 32.094 | 1.00 3 | | 6 |
| MOTA | | | GLN A | | | 38.479 | 36.541 | 33.480 | 1.00 4 | | 6 |
| ATOM | 618 | CD | | | | 38.574 | 35.755 | 34.426 | 1.00 4 | | .8 |
| ATOM | 619 | | GLN A | | | | 37.846 | 33.606 | 1.00 4 | | 7 |
| ATOM . | 620 | | GLN A | | | 38.703 | | 31.358 | 1.00 3 | | 6 |
| ATOM | 621 | C | GLN A | | | 37.561 | 32.920 | • | | | |
| MOTA | 622 | 0 | GLN A | | • | 36.732 | 33.598 | 30.760 | 1.00 3 | | 8 |
| MOTA | 623 | N | CYS A | | | 37.522 | 31.598 | 31.370 | 1.00 3 | | 7 |
| ATOM | 624 | CA | CYS A | 77 | | 36.511 | 30.862 | 30.627 | 1.00 3 | | 6 |
| MOTA | 625 | CB | CYS .A | 77 | | 37.187 | 30.181 | 29.454 | 1.00 3 | 10.25 | 6 |
| MOTA | 626 | SG | CYS A | 77. | | 38.479 | 29.071 | 30.044 | 1.00 3 | 33.94 | 16 |
| ATOM | 627 | C | CYS A | | | 35.851 | 29.795 | 31.498 | 1.00 3 | 1.97 | 6 |
| MOTA | 628 | ō | CYS A | | | 36.335 | 29.503 | 32.590 | 1.00 3 | 35.15 | 8 |
| | 629 | N | VAL A | | | 34.750 | 29.216 | 31.018 | 1.00 3 | 30.78 | 7 |
| ATOM | 630 | CA | VAL A | | | 34.069 | 28.139 | 31.747 | 1.00 3 | | 6 |
| MOTA | | | | | | 32.539 | 28.287 | 31.720 | 1.00 3 | | 6 |
| ATOM | 631 | CB | VAL A | | | 31.881 | 27.030 | 32.293 | 1.00 2 | | 6 |
| MOTA | 632 | | VAL A | | | | 29.503 | 32.526 | 1.00 | | 6 |
| ATOM | 633 | | VAL A | | | 32.129 | | | 1.00 2 | | 6 |
| ATOM . | 634 | С | VAL A | | | 34.420 | 26.794 | 31.110 | 1.00 2 | | 8 |
| MOTA | 635 | 0 | VAL A | | | 33.851 | 26.422 | 30.077 | | | 7 |
| MOTA | 636 | N | PRO A | | | 35.337 | 26.033 | 31.739 | 1.00 2 | | |
| ATOM | 637 | CD | PRO A | 79 | | 35.985 | 26.335 | 33.025 | 1.00 2 | | 6 |
| ATOM | 638 | CA | PRO A | 79 | | 35.793 | 24.724 | 31.261 | 1.00 2 | | 6 |
| ATOM | 639 | CB | PRO A | 79 | | 36.622 | 24.218 | 32.434 | 1.00 2 | | 6 |
| ATOM | 6.0 | CG | PRO A | 79 | | 37.239 | 25.500 | 32.922 | 1.00 2 | 25.68 | 6 |
| ATOM | 61 | С | PRO A | 79 | | 34.668 | 23.776 | 30.881 | 1.00 3 | 30.13 | 6 |
| MOTA | 6-2 | ō | PRO A | | | 33.697 | 23.624 | 31.615 | 1.00 | 30.87 | 8 |
| | 643 | N | LYS A | | | 34.796 | 23.136 | 29.727 | 1.00 3 | 33.44 | 7 |
| MOTA | 644 | CA | LYS A | | | 33.758 | 22.216 | 29.303 | 1.00 | 38.52 | 6 |
| MOTA | | | LYS A | | | 34.202 | 21.421 | 28.076 | 1.00 | | 6 |
| MOTA | 645 | CB | | | | 35.450 | 20.589 | 28.278 | 1.00 | | 6 |
| MOTA | 646 | CG | LYS A | | | | | | | | 6 |
| MOTA | 647 | CD | LYS A | | | 35.788 | 19.827 | 27.000 | 1.00 | | |
| ATOM | . 648 | CE | LYS A | 80 | | 37.035 | 18.976 | 27.168 | 1.00 | | 6 |
| ATOM | 649 | NZ | LYS A | 80 | - | 37.367 | 18.252 | 25.911 | 1.00 | | 7 |
| ATOM | 650 | С | LYS A | 80 | | 33.411 | 21.267 | 30.443 | 1.00 | | 6 |
| ATOM | 651 | 0 | LYS A | 80 | | 34.293 | 20.775 | 31.164 | 1.00 | | 8 |
| ATOM | 652 | N | GLY A | | | 32.112 | 21.035 | 30.602 | 1.00 | 32.57 | 7 |
| | 653 | CA | GLY A | | | 31.634 | 20.155 | 31.648 | 1.00 | 29.81 | 6 |
| ATOM | | C | GLY A | | | 31.477 | 20.884 | 32.965 | 1.00 | | 6 |
| ATOM | 654 | | | | | 30.544 | 20.612 | 33.723 | 1.00 | | 8 |
| ATOM | 655 | 0 | GLY A | | | | 21.830 | 33.218 | 1.00 | | 7 |
| ATOM | 656 | N | ALA A | | | 32.380 | | 34.458 | 1.00 | | 6 |
| MOTA | 657 | CA | ALA A | | | 32.384 | 22.602 | | 1.00 | | 6 |
| ATOM | 658 | CB | ALA A | | | 33.485 | 23.674 | 34.406 | - | | 6 |
| ATOM | 659 | С | ALA A | | | 31.066 | 23.245 | 34.886 | | 27.84 | |
| ATOM | 660 | 0 | ALA A | 82 | | 30.729 | 23.224 | 36.068 | 1.00 | 30.00 | 8 |
| | | | | | | | | - | | | |

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|-------------|-------------------|---|
| ATO1 | 4 661 N ARG A 83 | ** |
| ATON | | 30.310 23.811 33.951 1.00 31.15 7 |
| | 41. ILIG A 63 | |
| MOTA | 1 663 CB ARG A 83 | 54.345 I.UU 32 50 6 |
| ATOM | 664 55 | 28.285 24.941 33.127 1.00 37.19 6 |
| | THU A BO | 27 420 25 402 2.00 37.13 6 |
| ATOM | f 665 CD ARG A 83 | 33.400 1.00 47 77 |
| ATOM | 666 177 | 20.300 20.070 34 505 1 00 10 |
| | 14/G X 63 | 25 004 25 1.00 40.02 6 |
| ATOM | [667 00 | 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 |
| ATOM | | 67 0 10 27 4 AD 1 4 AD 1 AD 1 AD 1 AD 1 AD 1 AD 1 |
| | AUG A 03 | 24 640 00 |
| aTom. | 669 NH2 ARG A. 83 | |
| ATOM | 670 0 | |
| | | 20 200 22 524 2:00 20:03 / |
| MOTA | 671 O ARG A 83 | 33.103 I.UU 11 50 C |
| ATOM | 672 12 | 40.000 43.749 36 386 1 00 00 40 |
| | OLO A 04 | 27 640 22 424 |
| MOTA | 673 CA GLU A 94 | |
| ATOM | 674 00 | |
| | 45 GEO N 64 | 26 112 22 22 2 |
| MOTA | 675 CG GLU A 84 | 33.41/ 1.00 37 35 6 |
| ATOM | 576 CD 555 | 40.303 19.684 33.406 3.40 |
| | | 77 554 22 42 5 |
| MOTA | 677 OE1 GLU A 84 | 22.20/ 1.00 44 40 2 |
| MOTA | 678 OE2 GLU A 84 | 4/1/40 19.//1 11 202 1 00 44 44 |
| | | 77 676 64 45 4 |
| ATOM | 679 C GLUA 84 | 27 617 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM | 600 0 | 2,.01, 20.823 36.417 1 00 35 45 6 |
| | 1, 04 | 27.246 20.816 37 504 1.00 33.42 5 |
| MOTA | 681 N LYS A 85 | |
| ATOM | 602 02 | 20.727 20.226 36.002 1.00 35 21 7 |
| | 05 | 29.604 19.450 36.070 |
| MOTA | 683 CB LYS A 85 | 30.043 50.076 1.00 37.93 6 |
| MOTA | 604 00 | 30.041 19.030 36.076 1 00 40 61. |
| | 05 | |
| · ATOM | 685 CD LYS A 85 | 31 070 1.00 12.63 6 |
| ATOM | | 31.030 10.040 36.872 1.00.45 48 6 |
| | 05 | 32.054 15 523 37 070 |
| ATOM | 687 NZ LYS A 85 | 33 033 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM | COO ~ | 38,154 1.00 46,16 7 |
| ATOM | | 30.032 20 150 30 175 |
| | 689 O LYS A 85 | 20 161 10 51.00 37.00 6 |
| ATOM | 690 N TYR A 86 | 0.010 30.222 1.00 18 40 5 |
| ATOM | 601 63 | . 30.234 21.4/2 38.116 1 00 15 60 7 |
| | | 30 (71 00 1 |
| MOTA | 692 CB TYR A 86 | 27 751 00 |
| ATOM | 603 00 | 22.131 22.610 39.200 1 00 32 00 6 |
| | | |
| MOTA | 694 CD1 TYR A 86 | 22 420 25.222 4.00 33.63 6 |
| ATOM | 60E 000 | 33.120 20.393 39.932 1 00.33 13 6 |
| | 695 CEI TYR A 86 | |
| MOTA | 696 CD2 TYR A 86 | 22 020 22 22 22 22 22 22 22 22 22 22 22 |
| ATOM | 607 202 | |
| ATOM | | 34.645 20 178 37 633 3 68 |
| | 698 CZ TYR A 86 | |
| ATOM | 699 OH TYR A 86 | 35 434 |
| MOTA | | |
| | - 121 14 00 | 29.831 23.455 39.507 |
| ATOM | 701 O TYRA 86 | 30 100 30.21 6 |
| ATOM | 700 | |
| | | 28.712 23.594 38 893 1 60 60 |
| ATOM | 703 CA ASN A 87 | |
| ATOM | 704 CB ASN A 87 | |
| ATOM | 705 00 | 47.134 /4 618 /N /7N + AA |
| | | 25 22 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM | 706 OD1 ASN A 87 | 25 275 20.396 1.00 28.05 6 |
| ATOM | 707 | 23.2/3 23.4// 41.672 1.00 1 32 g |
| | ,, ,, | 75 434 96 000 no non |
| ATOM | 708 C ASN A 87 | 20 500 1 |
| ATOM | 709 O ASN A 87 | |
| ATOM | 710 | |
| | 710 N ILE A 88 | 20 545 |
| ATOM | 711 CA ILE A 88 | |
| ATOM | 11 00 | 37.809 1.00 33.77 6 |
| | | 31.894 26 774 37 776 |
| ATOM | 713 CG2 ILE A 88 | 22 25 25 |
| ATOM | 714 | 32.739 27.831 37.201 1.00 37.80 6 |
| | | 32.357 26.342 39 178 1 30 19 00 |
| ATOM | 715 CD1 ILE A 88 | 22 25 25 25 25 25 25 25 25 25 25 25 25 2 |
| ATOM | | 70 000 11.00 41.44 6 |
| | 717 | 30.083 27.857 36.482 1.00 32 20 6 |
| atom | 717 O ILE A 88 | 29 708 27 106 35 502 1.00 32.28 6 |
| ATOM | 718 N GLY A 89 | 20 22 23 23 25 25 26 27 28 |
| | 710 | 30.23/ 29.179 36.438 1.00 31 56 7 |
| ATOM | 719 CA GLY A 89 | 29.994 29.015 25.000 |
| ATOM | 720 C GLY A 89 | 20 505 33.207 1.00 30.82 6 |
| ATOM | 77. | 20.030 30.689 35.093 1.00 32 17 6 |
| | | 28.628 31.670 34.340 |
| MOTA | 722 N GLY A 90 | 27 670 30 357 35 35 30.42 8 |
| ATOM | | 37,670 30.257 35.821 1.00 31.51 7 |
| | 700 11 70 | /h (k/ 20 029 25 55 55 |
| atom · | 724 C GLY A . 90 | 26.316 32 346 36 534 1.00 32.32 |
| ATOM | 775 - | 2 |
| | 725 | 2/.302 32.671 37.129 1.00 33 97 9 |
| ATOM | 726 N TYR A 91 | |
| | | 25.144 32.882 36.504 1.00 33.88 7 |
| | | · - |

| ATOM | 727 | CA | TYR . | A 91 | 24.924 | 34.146 | 37.206 | 1.00 35.76 | 6 |
|--------|------------|-----|-------|--------|----------|----------|----------------|------------|-----|
| | | | | | | | | | |
| MOTA | 728 | CB | TYR . | A 91 | 23.465 | 34.589 | 37.058 | 1.00 38.10 | 6 |
| ATOM | 729 | CG | TYR . | A 91 | 23.089 | 35.733 | 37.990 | 1.00 42.40 | 6 |
| | | | | | | | - | | |
| ATOM | 730 | CDI | TYR . | A 91 | 23.417 | 37.057 | 37.688 | 1.00 43.57 | 6 |
| MOTA | 731 | CE1 | TYR . | A 91 | 23.105 | 38.106 | 38.5 77 | 1.00 42.44 | 6 |
| | | | | | | | | | |
| MOTA | 732 | CD2 | | | 22.444 | 35.484 | 39.205 | 1.00 44.07 | 6 |
| ATOM | 733 | CE2 | TYR . | A 91 | 22.132 | 36.526 | 40.097 | 1.00 42.67 | 6 |
| | | | | | | 37.825 | 39.775 | | |
| MOTA | 734 | CZ | TYR . | A 91 | 22.462 | | 39.113 | 1.00 42.41 | 6 |
| ATOM | 735 | OH | TYR . | A 91 | 22.130 | 38.835 | 40.646 | 1.00 43.69 | 8 |
| | 736 | C | TYR . | | 25.242 | 34.082 | 38.701 | 1.00 34.15 | 6 |
| ATOM | | | | | | | | | |
| MOTA | 737 | 0 | TYR . | A 91 | 25.821 | 35.014 | 39.266 | 1.00 29.52 | 8 |
| ATOM | 738 | N | GLU . | A 92 | 24.837 | 32.986 | 39.333 | 1.00 34.78 | 7 |
| | | | | | | | | | |
| ATOM · | 739 | CA | GLU . | A 92 | 25.024 | 32.797 | 40.767 | 1.00 38.46 | 6 |
| MOTA | 740 | CB | GLU A | A 92 | 24.233 | 31.564 | 41.211 | 1.00 43.99 | 6 |
| - | | | GLU : | | 23.932 | 31.489 | 42.700 | 1.00 52.10 | 6 |
| MOTA | 741 | CĠ | | | | | | | |
| ATOM | 742 | CD | GLU A | A 92 | 23.294 | 30.161 | 43.097 | 1.00 58.00 | 6 |
| ATOM | 743 | OE1 | GLU Z | A 92 | 24.001 | 29,126 | 43.058 | 1.00 60.63 | 8 |
| | | | | | | | | | |
| ATOM | 744 | OE2 | GLU A | A 92 | . 22.087 | 30.149 | 43.434 | 1.00 59.58 | 8 |
| ATOM | 745 | С | GLU A | A 92 | 26.492 | 32.669 | 41.208 | 1.00 36.42 | 5 |
| | 746 | Ō | GLU 2 | | 26.902 | 33.287 | 42.193 | 1.00 32.92 | 8 |
| ATOM | | | | | | | | | |
| ATOM | 747 | N | ASN A | A 93 | 27.280 | 31.883 | 40.473 | 1.00 34.12 | 7 |
| ATCM | 748 | CA | ASN 2 | A 93 | 28.693 | 31.671 | 40.808 | 1.00 33.24 | 6 |
| | | | | | | | | | 6 |
| ATOM | 749 | CB | ASN I | | 28.871 | 30.259 | 41.364 | 1.00 28.52 | |
| ATOM . | 750 | CG | ASN A | A 93 | 27.734 | 29.859 | 42.299 | 1.00 27.45 | 6 |
| ATOM | 751 | נתח | ASN 2 | A 93 | 27.547 | 30.457 | 43.355 | 1.00 21.76 | 8 |
| | | | | | | | | | |
| ATOM | 752 | ND2 | ASN A | A 93 | 26.956 | . 28.853 | 41.895 | 1.00 21.79 | 7 |
| MOTA | 753 | С | ASN A | A 93 | 29.529 | 31.843 | 39.535 | 1.00 35.04 | 6 |
| | 754 | | ASN 2 | | 30.160 | 30.898 | 39.059 | 1.00 33.81 | 8 |
| MOTA | | 0 | | | | | | | |
| ATOM | 755 | N | PRO 2 | A 94 | 29.583 | 33.081 | 39.01 0 | 1.00 36.19 | 7 |
| ATOM | 756 | CD | PRO 2 | A 94 | 28.970 | 34.231 | 39.690 | 1.00 34.62 | 6 |
| | - | | | | | | | | 6 |
| MOTA | 757 | CA | PRO I | | 30.274 | 33.560 | 37.808 | 1.00 34.80 | |
| ATOM | 758 | CB | PRO 2 | A. 94 | 29.924 | 35.050 | 37.791 | 1.00 33.94 | 6 |
| | 759 | CG | PRO A | A 94 | 28.619 | 35.095 | 38.516 | 1.00 36.13 | 6 |
| ATOM | | | | | | | | | |
| ATOM | 760 | С | PRO I | A 94 | . 31.775 | 33.379 | 37.733 | 1.00 34.63 | 6 |
| ATOM | 761 | 0 | PRO 2 | A 94 | 32.443 | 33.103 | 38.730 | 1.00 34.72 | 8 |
| ATOM | 762 | N | VAL 2 | A 95 | 32.299 | 33.556 | 36.526 | 1.00 33.57 | 7 |
| | | | | | | | | | 6 |
| ATOM | 763 | CA | VAL A | | 33.735 | 33.499 | 36.307 | 1.00 30.31 | |
| ATOM | 764 | CB | VAL A | A 95 | 34.085 | 33.171 | 34.841 | 1.00 29.88 | 6 |
| ATOM | 765 | CG1 | VAL 2 | A · 95 | 35.561 | 33.453 | 34.574 | 1.00 29.53 | 6 |
| | | | | | | | | 1.00 28.05 | 6 |
| MOTA | 766 | CG2 | VAL | | 33.795 | 31.713 | 34.563 | | |
| ATOM | 767 | С | VAL A | s 95 | 34.195 | 34.910 | 36.624 | 1.00 29.86 | 6 |
| | 768 | 0 | VAL 3 | A 95 | 33.524 | 35.879 | 36.272 | 1.00 29.07 | 8 |
| ATOM | | | | | | | | | |
| MOTA | 769 | N | SER A | A 96 | 35.318 | 35.019 | 37.317 | 1.00 30.89 | 7 |
| ATOM | 770 | CA | SER A | A 96 | 35.889 | 36.310 | 37.687 | 1.00 32.27 | 6 |
| | | | SER A | | 34.885 | 37.145 | 38.501 | 1.00 30.16 | 6 |
| ATOM | 771 | СВ | | | | | | | |
| MOTA | 772 | OG | SER 3 | 4 96 | 34.600 | 36.545 | 39.756 | 1.00 26.77 | 8 |
| MOTA | 773 | С | SER A | A 96 | 37.111 | 35.993 | 38.537 | 1.00 32.96 | 6 |
| | | | | | | | 38.511 | 1.00 33.77 | 8 |
| MOTA | 774 | 0 | SER 3 | A 96 | 37.603 | 34.865 | | | |
| ATOM | 775 | N | TYR A | s 97 | 37.609 | 36.973 | 39.282 | 1.00 32.66 | 7 |
| | 776 | CA | TYR A | | 38.753 | 36.712 | 40.132 | 1.00 31.95 | 6 |
| MOTA | | | | | | | | | |
| MOTA | 777 | CB | TYR A | 3 97 | 39.838 | 37.766 | 39.923 | 1.00 31.81 | 6 |
| ATOM | 778 | CG | TYR A | 97 | 40.416 | 37.729 | 38.525 | 1.00 30.39 | 6 |
| | | | | | | | | 1.00 30.63 | 6 |
| MOTA | 779 | | TYR A | | 39.820 | 38.434 | 37.479 | | |
| ATOM | 780 | CE1 | TYR A | 97 | 40.327 | 38.358 | 36.178 | 1.00 28.49 | 6 |
| | 781 | | TYR 2 | | 41.536 | 36.945 | 38.236 | 1.00 28.43 | 6 |
| ATOM | | | | | | | | | |
| ATOM | 782 | CE2 | TYR A | | 42.046 | 36.858 | 36.942 | 1.00 24.73 | 6 |
| ATOM | 783 | CZ | TYR A | 97 | 41.437 | 37.565 | 35.919 | 1.00 27.27 | 6 |
| | | | | | | _ | 34.633 | 1.00 26.70 | 8 |
| atom | 784 | OH | TYR A | | 41.915 | 37.455 | | | - |
| ATOM | 785 | C | TYR A | a 97 | 38.350 | 36,618 | 41.596 | 1.00 31.10 | 6 |
| | 786 | 0 | TYR A | | 39.178 | 36.735 | 42.495 | 1.00 33.01 | 8 |
| ATOM | | | | | | | | | . 7 |
| ATOM | 787 | N | ALA A | | 37.059 | 36.398 | 41.818 | 1.00 31.11 | |
| ATOM | 738 | CA | ALA A | 86 4 | 36.510 | 36.241 | 43.160 | 1.00 30.06 | 5 |
| | 789 | CB | ALA A | | 35.141 | 36.920 | 43.256 | 1.00 27.71 | 6 |
| ATOM | | | | | | | 43.357 | 1.00 31.24 | . 6 |
| ATCM | -90 | C . | ALA A | | 36.350 | 34.736 | | | |
| ATCM | 791 | 0 | ALA A | ¥ 98 | 36.335 | 34.238 | 44.487 | 1.00 29.66 | -8 |
| | 792 | N | MET A | | 36.249 | 34.030 | 42.230 | 1.00 29.50 | 7 |
| ATOM | , 54 | 44 | | | 30.243 | 54.000 | | | |

| ATOM 794 CB MET A 99 35.777 32.123 40.778 1.00 29.88 ATOM 795 CC MET A 99 35.972 32.123 40.778 1.00 29.78 ATOM 796 CC MET A 99 35.422 31.939 38.126 1.00 29.78 ATOM 797 CC MET A 99 35.422 31.939 31.800 42.783 1.00 29.78 ATOM 798 C MET A 99 35.422 31.939 31.800 42.783 1.00 29.78 ATOM 800 N PHE A 100 38.417 32.123 42.569 1.00 30.81 ATOM 801 CA PHE A 100 39.551 31.800 42.783 1.00 30.81 ATOM 801 CA PHE A 100 39.551 31.800 42.783 1.00 30.81 ATOM 803 CC PHE A 100 40.322 31.577 43.406 1.00 31.95 31.800 42.780 42.780 42.569 1.00 32.09 ATOM 803 CC PHE A 100 41.52 48.417 32.029 1.00 33.95 42.700 40.700 40.519 42.780 42.78 | ATC ATC | | 36.048 32.589 42.207 1.00 29 89 | |
|--|------------|---|------------------------------------|------------|
| ATOM 796 SD MET A 99 36.426 31.939 38.125 1.00 29.78 1 ATOM 797 CC MET A 99 35.629 30.273 38.347 1.00 29.78 1 ATOM 798 C MET A 99 37.199 31.800 42.783 1 1.00 29.78 1 ATOM 799 C MET A 99 37.199 31.800 42.783 1 1.00 29.78 1 ATOM 800 N PHE A 99 37.199 31.800 42.783 1 1.00 23.09 ATOM 801 CA PHE A 100 38.417 32.274 42.559 1 1.00 32.09 ATOM 802 CE PHE A 100 38.417 32.274 42.559 1 1.00 32.09 ATOM 803 CG PHE A 100 40.322 30.817 42.029 1 1.00 33.95 4 ATOM 803 CG PHE A 100 41.152 28.862 43.364 1 1.00 13.95 4 ATOM 805 CD2 PHE A 100 42.768 30.339 42.372 1 1.00 41.84 ATOM 805 CD2 PHE A 100 42.768 30.339 42.372 1 1.00 41.84 ATOM 807 CE2 PHE A 100 42.768 30.339 42.372 1 1.00 41.84 ATOM 807 CE2 PHE A 100 42.786 30.339 42.372 1 1.00 41.84 ATOM 809 C PHE A 100 42.786 30.339 42.372 1 1.00 41.84 ATOM 809 C PHE A 100 42.786 30.339 42.372 1 1.00 41.84 ATOM 809 C PHE A 100 42.786 30.339 42.372 1 1.00 41.84 ATOM 809 C PHE A 100 42.185 28.115 43.941 1 1.00 40.63 ATOM 809 C PHE A 100 43.517 28.487 43.729 1 1.00 39.89 6 ATOM 809 C PHE A 100 40.519 32.438 43.895 1 1.00 39.89 6 ATOM 811 N THR A 101 40.706 32.313 45.088 1 1.00 39.89 6 ATOM 812 CA THR A 101 42.063 34.261 43.969 1 1.00 22.48 ATOM 813 CB THR A 101 42.063 34.261 43.969 1 1.00 22.48 ATOM 815 CC THR A 101 42.063 34.261 43.969 1 1.00 22.48 ATOM 815 CC THR A 101 41.408 34.850 45.205 1 1.00 22.48 ATOM 815 CC THR A 101 41.408 34.850 45.205 1 1.00 22.99 ATOM 815 CC THR A 101 41.408 34.850 45.205 1 1.00 22.48 ATOM 820 C SER A 103 ATOM 810 C SER A 103 ATOM 821 C C SER A 103 ATOM 821 C C SER A 103 ATOM 822 C SER A 103 ATOM 823 C SER A 103 ATOM 823 C SER A 103 ATOM 824 C SER A 103 ATOM 825 C SER A 103 ATOM 826 C SER A 103 ATOM 827 C SER A 103 ATOM 828 C SER A 103 ATOM 829 C C SER A 103 ATOM 820 C SER A 103 ATOM 821 C SER A 103 ATOM 822 C SER A 103 ATOM 823 C SER A 103 ATOM 824 C SER A 103 ATOM 825 C SER A 103 ATOM 827 C SER | | OM 705 05 1161 A 99 | 35.774 32 123 40 770 1.00 29.89 | 9 |
| ATOM 797 CE MET A 99 36.426 31.939 38.126 1.00 25.78 1 ATOM 798 C MET A 99 35.629 30.273 38.347 1.00 25.05 ATOM 799 O MET A 99 36.993 31.800 42.783 1.00 30.59 1 ATOM 800 N PHE A 100 38.417 32.274 42.665 1.00 32.09 1 ATOM 801 CA PHE A 100 39.553 31.574 42.566 1.00 32.09 1 ATOM 802 CE PHE A 100 39.554 31.557 43.146 1.00 33.87 ATOM 803 CE PHE A 100 40.322 30.817 42.029 1.00 33.87 ATOM 804 CDI PHE A 100 41.434 29.979 42.578 1.00 41.14 1.00 33.87 ATOM 805 CEI PHE A 100 41.434 29.979 42.578 1.00 41.14 1.00 41.63 ATOM 805 CEI PHE A 100 42.765 80.339 42.372 1.00 42.18 ATOM 805 CEI PHE A 100 42.765 80.339 42.372 1.00 42.18 ATOM 805 CEI PHE A 100 43.805 29.600 42.944 1.00 41.63 6 ATOM 805 CEI PHE A 100 40.50 ATOM 807 CEI PHE A 100 40.766 3.30 39.89 6 ATOM 808 CZ PHE A 100 40.766 3.30 39.89 6 ATOM 808 CZ PHE A 100 40.766 3.30 30.231 45.088 1.00 33.98 6 ATOM 808 CZ PHE A 100 40.766 3.30 30.201 30.398 6 ATOM 809 CZ PHE A 100 40.766 3.30 30.201 30.398 6 ATOM 810 C PHE A 100 40.766 3.30 30.201 30.398 6 ATOM 812 CG THR A 101 41.137 33.415 43.245 1.00 38.21 6 ATOM 813 CB THR A 101 41.137 33.415 43.245 1.00 38.21 6 ATOM 814 CGI THR A 101 41.137 33.415 43.245 1.00 38.21 6 ATOM 815 CG THR A 101 41.488 48.60 45.205 1.00 33.98 6 ATOM 816 CG THR A 101 41.488 48.60 45.205 1.00 22.19 6 ATOM 816 CG THR A 101 41.488 48.60 45.205 1.00 22.38 8 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.19 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.19 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.382 8 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.382 8 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.257 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.257 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 102 39.503 35.374 45.000 22.248 6 ATOM 820 CG CHY A 100 44.448 52.351 | | M 706 on | 35.942 32.265 39 822 1.00 30.46 | 3 |
| ATOM 798 C MET A 99 37.199 30.273 38.347 1.00 25.05 1 ATOM 800 N PHE A 100 38.417 32.274 42.569 1.00 30.59 | | The op that H gg | 36.426 31.939 38.126 1.00 29.03 | |
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| ATOM 800 N PHE A 100 38.417 32.274 42.569 1.00 31.59 ATOM 800 CG PHE A 100 40.39.554 31.557 43.114 1.00 33.87 ATOM 800 CG PHE A 100 40.322 30.817 42.029 1.00 32.09 ATOM 800 CG PHE A 100 41.434 29.979 42.578 1.00 41.14 63 ATOM 800 CD PHE A 100 41.434 29.979 42.578 1.00 41.14 63 ATOM 800 CD PHE A 100 42.768 30.339 42.372 1.00 41.18 64 64 64 64 64 64 64 64 64 64 64 64 64 | OTA | M 700 0 1 33 | 37.199 31.800 42.783 1 00 20 01 |) |
| ATOM 801 CA PHE A 100 | ATO: | | 36.993 30.757 43.406 1.00 30 50 | . ! |
| ATOM 803 CG PHE A 100 | ATO: | M 801 CA PHE A 100 | 38.417 32.274 42.569 1.00 32 09 | |
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| ATOM 804 CD1 PHE A 100 ATOM 805 CD2 PHE A 100 ATOM 806 CEI PHE A 100 ATOM 807 CEE PHE A 100 ATOM 807 CEE PHE A 100 ATOM 807 CEE PHE A 100 ATOM 808 CZ PHE A 100 ATOM 809 CZ PHE A 100 ATOM 811 N THR A 101 ATOM 812 CA THR A 101 ATOM 813 CB THR A 101 ATOM 814 CG1 THR A 101 ATOM 815 CG2 THR A 101 ATOM 816 C THR A 101 ATOM 816 C THR A 101 ATOM 817 C THR A 101 ATOM 818 N SER A 103 ATOM 820 C GLY A 102 ATOM 821 O GLY A 102 ATOM 821 O GLY A 102 ATOM 821 O GLY A 102 ATOM 822 N SER A 103 ATOM 824 CE SER A 103 ATOM 825 C SER A 103 ATOM 826 C SER A 103 ATOM 827 O SER A 103 ATOM 828 N SER A 106 ATOM 839 CD LEU A 105 ATOM 830 CE SER A 104 ATOM 831 CE SER A 103 ATOM 830 C SER A 104 ATOM 831 C SER A 104 ATOM 832 C SER A 103 ATOM 827 O SER A 103 ATOM 828 N SER A 106 ATOM 839 CD LEU A 105 ATOM 831 C SER A 104 ATOM 831 C SER A 106 ATOM 842 C SER A 103 ATOM 831 C SER A 104 ATOM 831 C SER A 106 ATOM 831 C SER A 106 ATOM 831 C SER A 106 ATOM 831 C SER A 107 ATOM 832 C SER A 106 ATOM 833 C SER A 106 ATOM 834 C SER A 106 ATOM 835 C SER A 106 ATOM 836 C SER A 106 ATOM 837 C SER A 107 ATOM 848 C SER A 106 ATOM 849 C SER A 107 ATOM 840 C SER A 106 ATOM 841 C SER A 107 ATOM 841 C SER A 106 ATOM 842 C SER A 106 ATOM 843 C SER A 106 ATOM 845 C SER A 107 ATOM 846 C SER A 107 ATOM 847 N SER A 106 ATOM 848 C SER A 106 ATOM 849 C SER A 107 ATOM 840 C SE | | M 803 CG PHE A 100 | 41 434 20 22 42.029 1.00 33.95 | ì |
| ATOM 806 CEI PHE A 100 ATOM 807 CEI PHE A 100 ATOM 808 CE PHE A 100 ATOM 808 CE PHE A 100 ATOM 809 C PHE A 100 ATOM 809 C PHE A 100 ATOM 809 C PHE A 100 ATOM 800 CE PHE A 100 ATOM 800 CE PHE A 100 ATOM 800 CE PHE A 100 ATOM 810 O PHE A 100 ATOM 811 N THR A 101 ATOM 812 CA THR A 101 ATOM 813 CE THR A 101 ATOM 813 CG THR A 101 ATOM 816 C THR A 101 ATOM 815 CGZ THR A 101 ATOM 816 C THR A 101 ATOM 817 O THR A 101 ATOM 818 N GLY A 102 ATOM 819 CA GLY A 102 ATOM 820 C GLY A 102 ATOM 821 CA SER A 103 ATOM 821 CA SER A 103 ATOM 822 N SER A 103 ATOM 823 CA SER A 103 ATOM 824 CB SER A 103 ATOM 825 CG SER A 103 ATOM 826 C SER A 103 ATOM 827 O SER A 103 ATOM 828 N SER A 104 ATOM 830 CE SER A 104 ATOM 831 CG SER A 104 ATOM 832 CA SER A 104 ATOM 835 CG SER A 104 ATOM 836 CG SER A 105 ATOM 827 O SER A 104 ATOM 838 CD SER A 104 ATOM 839 CA SER A 104 ATOM 830 CE SER A 104 ATOM 830 CE SER A 104 ATOM 831 CG SER A 105 ATOM 830 CE SER A 104 ATOM 831 CG SER A 105 ATOM 830 CE SER A 104 ATOM 831 CG SER A 105 ATOM 830 CE SER A 104 ATOM 831 CG SER A 105 ATOM 835 CG SER A 106 ATOM 836 CG SER A 106 ATOM 837 CG LEU A 105 ATOM 838 CD LEU A 105 ATOM 838 CD LEU A 105 ATOM 838 CD LEU A 105 ATOM 836 CG SER A 104 ATOM 837 CG LEU A 105 ATOM 838 CD LEU A 105 ATOM 839 CG SER A 104 ATOM 830 CD SER A 104 ATOM 831 CG SER A 106 ATOM 831 CG SER A 107 ATOM 832 CA SER A 104 ATOM 834 C SER A 106 ATOM 835 CG SER A 106 ATOM 836 CG SER A 106 ATOM 837 CG LEU A 105 ATOM 838 CD LEU A 105 ATOM 838 CD LEU A 105 ATOM 839 CD SER A 104 ATOM 830 CD SER A 104 ATOM 830 CD SER A 106 ATOM 831 CG SER A 107 ATOM 832 CG SER A 106 ATOM 835 CG SER A 106 ATOM 836 CG SER A 106 ATOM 837 CG SER A 106 ATOM 838 CD SER A 106 ATOM 838 CD SER A 106 ATOM 838 CD SER A 106 ATOM 839 CD SER | | M 804 CD1 PHE A 100 | 41 152 22 42.578 1.00 41.14 | è |
| ATOM 807 CE2 PHE A 100 | | M 805 CD2 PHE A 100 | 42 760 20.002 43.364 1.00 41.84 | ė |
| ATOM 808 CZ PHE A 100 | | 806 CE1 PHE A 100 | 42 105 20 42.18 | ϵ |
| ATOM 810 C PHE A 100 | | TVP V TOO | 43.808 29.600 42.944 1.00.41.63 | . 6 |
| ATOM 810 O PHE A 100 | | 1111 X 100 | 43.517 28.487 43 729 1.00 40.50 | |
| ATOM 811 N THR A 101 41.137 33.415 43.245 1.00 28.219 6 ATOM 813 CB THR A 101 42.063 34.261 43.969 1.00 22.19 7 ATOM 814 CGI THR A 101 42.063 34.261 43.969 1.00 22.19 7 ATOM 815 CG THR A 101 43.441 34.795 42.052 1.00 22.88 6 ATOM 816 C THR A 101 43.441 34.795 42.052 1.00 21.99 8 ATOM 817 O THR A 101 41.408 36.335 43.876 1.00 15.00 6 ATOM 818 N GLY A 102 41.988 34.845 46.282 1.00 23.82 8 ATOM 820 C GLY A 102 40.197 35.377 46.231 1.00 21.71 6 ATOM 821 O GLY A 102 39.533 35.947 46.231 1.00 21.79 7 ATOM 821 O GLY A 102 39.533 35.947 46.231 1.00 21.23 6 ATOM 821 O GLY A 102 39.209 34.909 48.378 1.00 21.23 6 ATOM 822 N SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 824 CE SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 825 C SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 826 C SER A 103 37.454 31.598 46.314 1.00 22.01 8 ATOM 827 O SER A 103 39.188 32.040 48.032 1.00 23.773 8 ATOM 828 N SER A 104 40.364 32.099 43.914 1.00 30.61 8 ATOM 828 N SER A 104 40.364 32.099 47.410 1.00 30.61 8 ATOM 829 CS SER A 103 39.188 32.040 48.032 1.00 28.76 7 ATOM 820 CS SER A 103 39.188 37.091 49.620 1.00 22.71 8 ATOM 830 CB SER A 104 42.769 31.683 47.099 1.00 28.76 6 ATOM 831 O SER A 104 42.769 31.683 47.099 1.00 28.76 6 ATOM 833 C SER A 104 42.769 31.683 47.099 1.00 28.77 6 ATOM 834 C LEU A 105 41.890 33.705 48.896 1.00 23.91 7 ATOM 835 C LEU A 105 41.890 37.75 50.338 1.00 23.01 8 ATOM 836 CB LEU A 105 41.890 37.75 50.338 1.00 23.01 8 ATOM 840 C LEU A 105 41.890 37.75 50.388 1.00 23.01 6 ATOM 841 O LEU A 105 41.890 37.75 50.388 1.00 23.01 6 ATOM 842 C SER A 104 30.54 42.501 34.485 50.391 1.00 23.67 6 ATOM 846 C ALEU A 105 41.890 37.75 50.388 1.00 25.77 6 ATOM 847 N THR A 107 39.602 31.897 50.338 1.00 25.77 6 ATOM 848 C ALEU A 105 41.890 33.186 50.008 1.00 23.01 6 ATOM 842 C ALEU A 105 41.890 33.186 50.008 1.00 23.01 6 ATOM 843 C ALA A 106 38.893 33.186 50.008 1.00 23.01 6 ATOM 846 C ALA A 106 38.953 33.186 50.008 1.00 23.07 6 ATOM 847 N THR A 107 39.602 30.760 52.754 1.00 22.38 6 ATOM 858 N SER A 109 43.227 50.00 50.00 60.00 28.57 | | - 1 TUL A 100 | 40.519 32.438 43.895 1.00 33.89 | |
| ATOM 812 CA THR A 101 42.063 34.261 43.969 1.00 22.19 6 ATOM 813 CB THR A 101 42.063 35.378 43.072 1.00 22.48 6 ATOM 816 C THR A 101 43.441 34.795 42.052 1.00 22.48 6 ATOM 816 C THR A 101 43.441 34.795 42.052 1.00 22.48 6 ATOM 816 C THR A 101 41.408 34.860 45.205 1.00 21.79 7 ATOM 818 N GLY A 102 40.197 35.377 45.068 1.00 21.79 7 ATOM 819 CA GLY A 102 39.533 35.947 45.068 1.00 21.79 7 ATOM 820 C GLY A 102 39.533 35.947 45.068 1.00 21.79 7 ATOM 821 N SER A 103 38.512 33.792 46.541 1.00 23.03 6 ATOM 822 N SER A 103 38.512 33.792 46.541 1.00 22.59 7 ATOM 823 CA SER A 103 38.512 33.792 46.541 1.00 22.59 7 ATOM 824 CB SER A 103 38.512 33.792 46.541 1.00 22.59 7 ATOM 825 OG SER A 103 37.454 31.598 46.314 1.00 28.10 6 ATOM 828 N SER A 103 36.314 32.099 45.639 1.00 32.01 8 ATOM 829 CA SER A 103 39.188 32.040 48.032 1.00 23.03 6 ATOM 828 N SER A 103 39.188 32.040 48.032 1.00 23.03 6 ATOM 828 N SER A 103 39.188 32.040 48.032 1.00 27.73 6 ATOM 830 CS SER A 104 41.590 31.554 49.144 1.00 30.61 8 ATOM 830 CS SER A 104 41.590 31.555 48.008 1.00 23.57 6 ATOM 831 CG SER A 104 42.769 31.663 47.039 1.00 23.57 6 ATOM 833 CS SER A 104 42.769 31.663 47.039 1.00 23.57 6 ATOM 834 C SER A 104 42.769 31.653 44.99 49.261 1.00 23.57 6 ATOM 836 CB LEU A 105 41.990 33.705 48.986 1.00 23.57 6 ATOM 837 CG LEU A 105 41.990 33.705 48.986 1.00 23.57 6 ATOM 841 O LEU A 105 41.909 33.705 48.986 1.00 23.57 6 ATOM 842 N ALEU A 105 41.909 33.705 48.986 1.00 23.57 6 ATOM 843 CA LEU A 105 41.909 33.705 48.986 1.00 23.57 6 ATOM 846 CA LEU A 105 41.604 34.448 52.331 1.00 21.60 8 ATOM 848 CA THR A 107 39.608 37.471 34.423 51.358 1.00 22.75 8 ATOM 848 CA THR A 107 39.608 37.471 34.423 51.358 1.00 22.75 8 ATOM 848 CA THR A 107 39.608 37.471 34.423 51.358 1.00 22.75 8 ATOM 848 CA THR A 107 39.608 37.471 34.423 51.358 1.00 22.75 8 ATOM 848 CA THR A 107 39.608 37.471 34.423 51.358 1.00 22.75 8 ATOM 855 C GLY A 108 43.247 31.187 53.718 1.00 28.56 7 ATOM 856 C GLY A 108 43.247 31.187 53.718 1.00 28.56 7 ATOM 856 C GLY A 108 43.247 31.187 53.718 1.00 28.56 7 ATOM | ATOM | 11 100 | 40.706 32.231 45.088 1.00 38.33 | |
| ATOM 813 CB THR A 101 | ATOM | 7 101 | 41.13/ 33.415 43.245 1.00 28 00 | |
| ATOM 815 CG 27 THR A 101 | ATOM | 813 CB THR A 101 | 43 603 34.201 43.969 1.00 22 19 | |
| ATOM 816 C THR A 101 | | 814 OG1 THR A 101 | 43 441 24 700 43.072 1.00 22.48 | |
| ATOM 816 C THR A 101 41.408 34.860 45.205 1.00 21.707 6 7 7 7 7 8 7 8 8 8 8 8 8 8 8 8 8 9 9 9 9 | | 815 CG2 THR A 101 | 43 469 26 25 42.052 1.00 21.99 | |
| ATOM 819 C. GLY A 102 40.197 35.377 45.068 1.00 21.79 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 | | 816 C THR A 101 | 41 400 34.333 43.876 1.00 15.00 | |
| ATOM 820 C GLY A 102 39.533 35.947 46.231 1.00 21.23 6 ATOM 821 O GLY A 102 39.533 35.947 46.231 1.00 21.23 6 ATOM 822 N SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 823 CA SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 824 CE SER A 103 38.6512 33.792 46.544 1.00 22.59 7 ATOM 825 OG SER A 103 37.454 31.598 46.314 1.00 28.10 6 ATOM 825 OG SER A 103 37.454 31.598 46.314 1.00 28.10 6 ATOM 826 C SER A 103 39.188 32.040 48.032 1.00 27.73 6 ATOM 827 O SER A 103 39.188 32.040 48.032 1.00 27.73 6 ATOM 828 N SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 829 C SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 830 CB SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 831 OG SER A 104 42.501 31.044 45.804 1.00 28.76 7 ATOM 832 C SER A 104 42.501 31.044 45.804 1.00 23.01 8 ATOM 835 CA LEU A 105 42.063 31.897 50.338 1.00 22.51 7 ATOM 836 CB LEU A 105 42.261 33.705 48.986 1.00 23.57 6 ATOM 837 CG LEU A 105 44.502 31.689 50.008 1.00 23.57 6 ATOM 839 CD2 LEU A 105 44.502 36.551 49.178 1.00 23.57 6 ATOM 840 C LEU A 105 44.502 36.551 49.178 1.00 23.48 6 ATOM 840 C LEU A 105 44.502 36.551 49.178 1.00 23.57 6 ATOM 841 O LEU A 105 44.502 36.551 49.178 1.00 23.57 6 ATOM 842 CA ALA A 106 39.088 31.58 43.159 1.00 23.57 6 ATOM 844 CB ALA A 106 39.088 33.158 52.390 1.00 23.57 6 ATOM 845 CA ALA A 106 39.088 33.158 52.390 1.00 23.57 6 ATOM 846 CA ALA A 106 39.088 33.158 52.390 1.00 23.57 6 ATOM 846 CA ALA A 106 39.088 33.158 52.290 1.00 23.57 6 ATOM 847 N THR A 107 39.402 39.403 31.595 52.756 6 ATOM 848 CA THR A 107 39.403 32.057 52.111 1.00 25.65 7 ATOM 840 C THR A 107 39.403 32.505 52.387 1.00 25.32 7 ATOM 840 CA ALA A 106 39.088 33.158 52.290 1.00 23.48 6 ATOM 845 CA ALA A 106 39.088 33.158 54.002 52.754 1.00 25.56 7 ATOM 848 CA THR A 107 39.403 32.057 52.111 1.00 25.65 7 ATOM 848 CA THR A 107 39.706 29.637 51.111 1.00 25.65 7 ATOM 840 CA ALA A 106 39.088 33.158 54.002 52.754 1.00 22.75 8 ATOM 850 CG THR A 107 39.706 29.637 51.711 1.00 25.65 7 ATOM 850 CG THR A | | - 1111 X 101 | 41.988 34.845 46 383 1.00 21.71 | 6 |
| ATOM 820 C GLY A 102 39.072 34.833 47.153 1.00 23.03 6 820 X SER A 103 39.209 34.999 48.378 1.00 20.41 8 7 ATOM 822 CB SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 826 CC SER A 103 37.454 31.598 46.314 1.00 22.59 7 ATOM 827 O SER A 103 37.454 31.598 46.314 1.00 22.59 7 ATOM 827 O SER A 103 39.188 32.040 48.032 1.00 27.73 6 8 ATOM 827 O SER A 103 39.189 32.040 48.032 1.00 27.73 6 ATOM 829 CA SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 830 CB SER A 104 41.590 31.552 48.008 1.00 28.55 6 ATOM 831 OG SER A 104 42.769 31.683 47.039 1.00 28.74 6 ATOM 832 C SER A 104 42.769 31.683 47.039 1.00 28.75 6 ATOM 833 O SER A 104 42.769 31.693 7.00 32.01 8 ATOM 833 C SER A 104 42.265 31.897 50.338 1.00 25.17 8 ATOM 835 CA LEU A 105 42.049 36.082 49.382 1.00 25.17 8 ATOM 836 CB LEU A 105 42.049 36.082 49.382 1.00 23.91 7 ATOM 838 CD1 LEU A 105 44.502 36.551 49.178 1.00 23.36 6 ATOM 844 CB ALE A 105 41.870 32.401 49.226 1.00 25.67 6 ATOM 839 CD2 LEU A 105 42.163 34.698 50.008 1.00 23.91 7 ATOM 836 CB LEU A 105 42.163 34.698 50.008 1.00 23.91 7 ATOM 836 CB LEU A 105 44.502 36.551 49.178 1.00 22.38 6 ATOM 844 CB ALE A 105 41.870 32.401 49.226 1.00 25.67 6 ATOM 845 CA LEU A 105 41.870 32.401 49.226 1.00 25.67 6 ATOM 846 CB LEU A 105 44.502 36.551 49.178 1.00 22.38 6 ATOM 846 CB LEU A 105 44.502 36.551 49.178 1.00 23.39 7 ATOM 848 CB LEU A 105 44.502 36.551 49.178 1.00 22.38 6 ATOM 845 CB ALE A 106 37.471 34.423 51.358 1.00 22.75 8 ATOM 846 CB ALE A 106 37.471 34.423 51.358 1.00 22.75 8 ATOM 846 CB ALE A 106 37.471 34.423 51.358 1.00 22.75 8 ATOM 847 N THR A 107 39.706 29.688 50.868 1.00 22.75 8 ATOM 849 CB THR A 107 39.706 29.688 50.868 1.00 22.75 8 ATOM 849 CB THR A 107 39.706 29.688 50.868 1.00 22.75 8 ATOM 849 CB THR A 107 39.706 29.688 50.868 1.00 22.75 8 ATOM 850 CG LTH A 107 39.706 29.688 50.868 1.00 22.55 6 ATOM 850 CG LTH A 107 39.706 29.688 50.868 1.00 22.75 8 ATOM 855 CA GLY A 108 43.027 31.991 55.019 1.00 30.26 6 ATOM 855 CA GLY A 108 43.027 31.499 55.076 1.00 32.807 8 ATOM 855 N N SER A 109 30.25 55.076 1.00 32. | | . OD1 A 102 | 40 102 25 25 202 1.00 43.82 | |
| ATOM 821 O GLY A 102 39.072 34.833 47.153 1.00 23.03 6 ATOM 822 N SER A 103 38.512 33.792 46.534 1.00 22.59 7 ATOM 823 CA SER A 103 38.512 33.792 46.544 1.00 22.59 7 ATOM 825 OG SER A 103 36.314 32.099 45.639 1.00 32.01 8 ATOM 826 C SER A 103 36.314 32.099 45.639 1.00 32.01 8 ATOM 827 O SER A 103 39.188 32.040 48.032 1.00 27.73 6 ATOM 828 N SER A 104 40.364 32.080 47.410 1.00 30.61 8 ATOM 829 CA SER A 104 41.590 31.552 48.008 1.00 28.76 7 ATOM 830 CB SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 832 C SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 833 O SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 835 CA LEU A 105 42.063 31.683 47.091 49.672 1.00 25.57 6 ATOM 836 CB LEU A 105 42.163 36.695 50.008 1.00 23.91 7 ATOM 837 CG LEU A 105 42.163 36.695 50.008 1.00 23.91 7 ATOM 838 CD1 LEU A 105 44.502 31.897 50.338 1.00 25.17 8 ATOM 839 CD2 LEU A 105 42.163 36.695 50.008 1.00 23.91 7 ATOM 836 CB LEU A 105 44.502 31.897 50.338 1.00 25.17 8 ATOM 837 CG LEU A 105 42.163 36.695 50.008 1.00 23.91 7 ATOM 838 CD1 LEU A 105 44.502 31.897 50.338 1.00 25.17 8 ATOM 840 C LEU A 105 44.502 31.897 50.338 1.00 25.17 8 ATOM 841 O LEU A 105 44.502 31.897 50.338 1.00 25.17 8 ATOM 842 N ALA A 106 39.088 33.158 57.091 49.672 1.00 25.50 6 ATOM 841 C ALA A 106 39.088 33.158 50.008 1.00 23.91 7 ATOM 842 C ALA A 106 39.088 33.158 50.008 1.00 23.51 6 ATOM 847 N THR A 107 39.706 29.637 51.182 1.00 23.48 6 ATOM 849 C S THR A 107 39.706 29.637 51.131 1.00 21.50 8 ATOM 849 C S THR A 107 39.706 29.637 51.713 1.00 25.55 6 ATOM 849 C S THR A 107 39.706 29.637 51.713 1.00 25.55 6 ATOM 849 C S THR A 107 39.706 29.637 51.713 1.00 25.55 6 ATOM 849 C S THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 850 C THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 850 C GLY A 108 43.227 31.191 55.019 1.00 28.57 6 ATOM 851 C GLY A 108 43.227 31.499 55.009 1.00 28.57 6 ATOM 855 C GLY A 108 43.227 31.499 55.009 1.00 28.57 6 ATOM 858 N SER A 109 30.00 30.266 6 ATOM 858 N SER A 109 30.00 30.2 | | CII. GD1 A 102 | 39.533 35.947 46 231 1 20 21.79 | |
| ATOM 822 N SER A 103 38.512 33.792 46.544 1.00 20.41 8 38.70M 824 CB SER A 103 37.454 31.598 46.314 1.00 28.10 6 ATOM 825 OG SER A 103 37.454 31.598 46.314 1.00 28.10 6 ATOM 826 C SER A 103 39.188 32.090 48.032 1.00 27.73 6 ATOM 827 O SER A 103 39.188 32.090 48.032 1.00 27.73 6 ATOM 828 N SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 830 CB SER A 104 41.590 31.552 48.008 1.00 28.76 6 ATOM 832 C SER A 104 42.501 31.044 45.804 1.00 30.61 8 ATOM 832 C SER A 104 41.870 32.401 49.226 1.00 28.75 6 ATOM 833 CB SER A 104 41.870 32.401 49.226 1.00 25.57 6 ATOM 836 CB LEU A 105 41.800 33.705 48.986 1.00 25.17 8 ATOM 836 CB LEU A 105 42.163 34.698 50.008 1.00 23.91 7 ATOM 838 CD1 LEU A 105 42.163 34.698 50.008 1.00 23.91 7 ATOM 839 CD2 LEU A 105 42.163 37.091 49.672 1.00 23.57 6 ATOM 840 C LEU A 105 44.502 36.551 49.178 1.00 22.388 6 ATOM 841 O LEU A 105 41.870 34.448 52.331 1.00 21.50 8 ATOM 841 C LEU A 105 41.870 34.448 52.331 1.00 22.388 6 ATOM 844 CB ALA A 106 38.884 34.423 51.957 1.00 23.48 6 ATOM 845 C ALA A 106 38.894 34.423 51.358 1.00 22.75 8 ATOM 846 C ALA A 106 38.895 33.158 52.790 1.00 25.57 6 ATOM 846 C ALA A 106 38.895 33.158 52.790 1.00 25.56 6 ATOM 847 N THR A 107 39.410 32.07 65 52.32 7 ATOM 848 CA THR A 107 39.410 32.07 65 52.37 7 ATOM 848 CA THR A 107 39.410 32.07 65 52.38 1.00 24.28 6 ATOM 847 N THR A 107 39.410 32.07 65 52.57 6 ATOM 847 N THR A 107 39.410 32.07 65 52.57 6 ATOM 848 CA THR A 107 39.410 32.07 65 52.57 6 ATOM 849 CB THR A 107 39.410 32.07 65 52.57 6 ATOM 849 CB THR A 107 39.410 32.07 65 52.58 6 ATOM 855 C GLY A 108 43.247 31.187 53.718 1.00 25.56 6 ATOM 856 C GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 856 C GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 856 N G GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 858 N SER A 109 43.207 31.921 55.019 1.00 32.66 6 ATOM 858 N SER A 109 43.207 31.921 55.019 1.00 32.66 6 ATOM 858 N SER A 109 43.207 31.921 55.019 1.00 32.66 6 ATOM 858 N SER A 109 43.207 31.921 55.019 1.00 32.98 8 | | - C GD1 A 102 | 39.072 34.833 47.153 1 00 23 03 | |
| ATOM 823 CA SER A 103 38.028 32.640 47.276 1.00 22.559 7 ATOM 825 OG SER A 103 36.314 32.099 45.639 1.00 32.01 8 32.040 827 O SER A 103 39.188 32.040 48.032 1.00 27.73 6 32.040 47.410 1.00 28.76 7 32.040 48.032 1.00 28.76 7 32.040 48.032 1.00 28.76 7 32.040 48.032 1.00 28.76 7 32.040 48.040 49.144 1.00 30.61 8 40.040 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.144 1.00 30.61 8 40.054 49.054 49.055 49.055 49.055 6 40.055 49. | ATOM | 822 N SER A 103 | 48.378 1.00 20 41 | |
| ATOM 824 CB SER A 103 37.454 31.598 46.314 1.00 26.51 6 ATOM 825 CG SER A 103 36.314 32.099 45.639 1.00 32.01 8 ATOM 827 O SER A 103 39.188 32.040 48.032 1.00 27.73 6 ATOM 828 N SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 830 CB SER A 104 41.590 31.552 48.008 47.410 1.00 28.76 7 ATOM 831 OG SER A 104 42.769 31.663 47.039 1.00 28.75 6 ATOM 832 C SER A 104 42.769 31.663 47.039 1.00 28.55 6 ATOM 833 O SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 833 O SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 835 CA LEU A 105 42.026 31.897 50.338 1.00 25.57 6 ATOM 836 CB LEU A 105 42.163 34.698 50.008 1.00 23.01 6 ATOM 837 CG LEU A 105 42.163 34.698 50.008 1.00 23.01 6 ATOM 838 CD1 LEU A 105 43.158 37.091 49.672 1.00 26.30 6 ATOM 840 C LEU A 105 41.870 32.481 49.174 1.00 22.38 6 ATOM 841 O LEU A 105 41.870 32.481 49.174 1.00 22.38 6 ATOM 842 N ALA A 106 39.887 34.555 50.381 1.00 27.36 6 ATOM 843 CA ALA A 106 39.887 34.555 50.897 1.00 22.38 7 ATOM 844 CB ALA A 106 39.887 34.555 50.897 1.00 22.38 6 ATOM 847 N THR A 107 39.620 30.760 52.754 1.00 25.557 6 ATOM 848 CA THR A 107 39.620 30.760 52.754 1.00 25.557 6 ATOM 849 CB THR A 107 39.620 30.760 52.754 1.00 25.557 6 ATOM 849 CB THR A 107 39.620 30.760 52.754 1.00 25.557 6 ATOM 849 CB THR A 107 39.620 30.760 52.754 1.00 25.557 6 ATOM 849 CB THR A 107 39.620 30.760 52.754 1.00 25.55 6 ATOM 849 CB THR A 107 39.620 30.760 52.754 1.00 25.554 6 ATOM 855 CG GLY A 108 43.247 31.187 53.718 1.00 21.92 6 ATOM 855 C GLY A 108 43.207 31.921 55.019 1.00 28.37 6 ATOM 855 C GLY A 108 43.207 31.921 55.019 1.00 28.37 6 ATOM 855 N SER A 104 43.502 31.499 55.019 1.00 30.266 6 ATOM 855 N SER A 104 40.354 31.99 55.019 1.00 30.266 6 ATOM 855 N SER A 104 40.364 32.208 31.499 55.019 1.00 30.266 6 ATOM 855 N SER A 108 43.502 31.499 55.019 1.00 30.266 6 ATOM 855 N SER A 108 43.502 31.499 55.019 1.00 30.266 6 ATOM 855 N SER A 108 43.502 31.499 55.019 1.00 30.266 6 ATOM 855 N SER A 108 43.502 31.499 55.019 1.00 30.266 6 ATOM 855 N SER A 104 40.364 32.208 31.499 55.019 1.00 30.266 6 ATOM 855 N SER | | 823 CA SER A 103 | 30 030 33.792 46.544 1.00 22.59 | |
| ATOM 825 CG SER A 103 36.314 32.099 45.639 1.00 32.01 8 36.314 32.099 45.639 1.00 32.01 8 39.188 32.040 48.032 1.00 27.73 6 37.00 32.01 8 39.188 32.040 48.032 1.00 27.73 6 37.00 32.01 8 39.188 32.040 48.032 1.00 27.73 6 37.00 32.01 8 39.188 32.040 48.032 1.00 27.73 6 37.00 32.01 8 39.188 32.040 48.032 1.00 27.73 6 37.00 32.00 47.00 30.61 8 39.00 32.00 47.00 30.61 8 37.00 32.00 47.00 30.61 8 37.00 32.00 47.00 30.61 8 37.00 32.00 47.00 30.61 8 37.00 32.00 47.00 30.61 8 37.00 32.00 47.00 30.61 8 37.00 32.00 | | 824 CB SER A 103 | 37 454 32 52.040 47.276 1.00 26.51 | |
| ATOM 827 O SER A 103 ATOM 828 N SER A 103 ATOM 829 CA SER A 104 ATOM 830 CB SER A 104 ATOM 831 OG SER A 104 ATOM 832 C SER A 104 ATOM 833 CB SER A 104 ATOM 834 C SER A 104 ATOM 835 CA LEU A 105 ATOM 836 CB LEU A 105 ATOM 837 CB LEU A 105 ATOM 838 CD1 LEU A 105 ATOM 838 CD1 LEU A 105 ATOM 839 CD2 LEU A 105 ATOM 840 C LEU A 105 ATOM 841 O LEU A 105 ATOM 841 O LEU A 105 ATOM 842 N ALA A 106 ATOM 843 CA ALA A 106 ATOM 844 CB ALA A 106 ATOM 845 C ALA A 106 ATOM 846 O ALA A 106 ATOM 847 N THR A 107 ATOM 848 CA THR A 107 ATOM 848 CA THR A 107 ATOM 849 CB THR A 107 ATOM 855 CA GLY A 108 ATOM 855 N SER A 109 ATOM 855 N SER A 109 ATOM 855 N SER A 109 ATOM 855 N SER A 104 A1.870 32.401 A1.590 31.552 A8.080 47.410 1.00 28.75 A2.080 47.410 1.00 22.68 A7.090 31.582 A8.081 47.039 1.00 28.55 A8.080 47.039 1.00 28.75 A8.080 47.039 1.00 28.75 A8.080 47.039 1.00 28.75 A8.080 47.039 1.00 28.75 B8.080 47.039 1.00 28.75 B8.080 47.039 1.00 23.01 B8.080 47.039 1.00 28.75 B8.080 49.382 1.00 22.38 B8.080 49.382 1.00 22.75 B8.080 49.382 1.00 22.75 B8.080 49.382 1.00 22.75 B8.080 49.382 1.00 28.51 ATOM 855 N GLY A 108 A3.027 31.995 B8.02 1.00 22.75 | | 825 OG SER A 103 | 36 314 32.398 46.314 1.00 28.10 | |
| ATOM 828 N SER A 104 ATOM 829 CA SER A 104 ATOM 830 CB SER A 104 ATOM 831 OG SER A 104 ATOM 832 C SER A 104 ATOM 833 OG SER A 104 ATOM 834 N LEU A 105 ATOM 835 CA LEU A 105 ATOM 836 CB LEU A 105 ATOM 837 CG LEU A 105 ATOM 838 CD1 LEU A 105 ATOM 838 CD1 LEU A 105 ATOM 839 CD2 LEU A 105 ATOM 839 CD2 LEU A 105 ATOM 840 C LEU A 105 ATOM 841 O LEU A 105 ATOM 841 O LEU A 105 ATOM 842 N ALA A 106 ATOM 842 N ALA A 106 ATOM 845 C ALA A 106 ATOM 845 C ALA A 106 ATOM 846 O ALA A 106 ATOM 847 N THR A 107 ATOM 848 CA THR A 107 ATOM 848 CA THR A 107 ATOM 849 CB THR A 107 ATOM 851 CG2 THR A 107 ATOM 852 C THR A 107 ATOM 853 O THR A 107 ATOM 855 CA GLY A 108 ATOM 857 O GLY A 108 ATOM 858 N SER A 104 A1.85 SER A 104 A0.364 32.080 47.410 1.00 28.75 7 7 840.31.552 48.008 1.00 28.75 7 7 841.604 42.769 31.683 47.039 1.00 25.54 6 42.049 31.693 47.039 1.00 25.57 6 81.002 25.57 6 82.401 49.226 1.00 25.67 6 82.401 49.226 1.00 25.67 6 82.401 49.226 1.00 25.67 6 82.402 31.897 50.338 1.00 25.17 8 84.986 1.00 23.91 7 84.502 36.551 49.178 1.00 23.59 6 8 8 8 8.413 4.698 50.082 1.00 23.91 7 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 | | - 55% 7 103 | 39.188 32.040 48.033 1.00 32.01 | |
| ATOM 829 CA SER A 104 40.364 32.080 47.410 1.00 28.76 7 ATOM 830 CB SER A 104 42.769 31.552 48.008 1.00 28.75 6 ATOM 831 OG SER A 104 42.769 31.683 47.039 1.00 28.74 6 ATOM 832 C SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 833 O SER A 104 42.826 31.897 50.338 1.00 25.57 6 ATOM 834 N LEU A 105 41.909 33.705 48.986 1.00 25.17 8 ATOM 835 CA LEU A 105 42.049 36.082 49.382 1.00 23.91 7 ATOM 836 CB LEU A 105 42.049 36.082 49.382 1.00 23.57 6 ATOM 838 CD1 LEU A 105 42.049 36.082 49.382 1.00 23.57 6 ATOM 839 CD2 LEU A 105 44.502 36.551 49.178 1.00 23.36 6 ATOM 840 C LEU A 105 44.502 36.551 49.178 1.00 27.36 6 ATOM 841 O LEU A 105 41.187 34.559 51.182 1.00 27.36 6 ATOM 842 N ALA A 106 39.887 34.556 50.897 1.00 25.32 7 ATOM 844 CB ALA A 106 39.887 34.556 50.897 1.00 25.32 7 ATOM 844 CB ALA A 106 39.887 34.423 51.358 1.00 21.50 8 ATOM 845 C ALA A 106 39.887 34.423 51.358 1.00 22.75 8 ATOM 846 O ALA A 106 38.884 34.423 51.358 1.00 22.75 8 ATOM 847 N THR A 107 39.400 39.706 52.754 1.00 25.54 6 ATOM 848 CA THR A 107 39.410 32.057 52.111 1.00 25.65 7 ATOM 848 CA THR A 107 39.620 30.760 52.754 1.00 25.54 6 ATOM 850 OGI THR A 107 39.706 29.637 51.713 1.00 25.55 7 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 21.66 6 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 25.54 6 ATOM 855 C GLY A 108 43.247 31.191 52.996 1.00 28.57 6 ATOM 855 C GLY A 108 43.247 31.191 52.996 1.00 28.57 6 ATOM 857 O GLY A 108 43.247 31.191 52.996 1.00 28.57 6 ATOM 858 N SER A 104 42.501 31.499 55.076 1.00 32.98 8 | | - -: . 11 103 | 30 010 25 50 50 50 2 1.00 27.73 | |
| ATOM 830 CB SER A 104 42.769 31.552 48.008 1.00 28.55 6 ATOM 831 OG SER A 104 42.769 31.683 47.039 1.00 28.74 6 ATOM 832 C SER A 104 42.501 31.044 45.804 1.00 35.04 8 ATOM 833 O SER A 104 42.026 31.897 50.338 1.00 25.57 6 ATOM 834 N LEU A 105 41.909 33.705 48.986 1.00 25.57 6 ATOM 835 CA LEU A 105 42.049 36.082 49.382 1.00 23.91 7 ATOM 836 CB LEU A 105 42.049 36.082 49.382 1.00 23.57 6 ATOM 838 CD1 LEU A 105 43.158 37.091 49.672 1.00 26.30 6 ATOM 838 CD1 LEU A 105 44.502 36.551 49.178 1.00 23.36 6 ATOM 840 C LEU A 105 44.502 36.551 49.178 1.00 27.36 6 ATOM 841 O LEU A 105 41.187 34.559 51.182 1.00 23.48 6 ATOM 842 N ALA A 106 39.887 34.556 50.897 1.00 25.32 7 ATOM 844 CB ALA A 106 39.887 34.555 50.897 1.00 26.04 6 ATOM 845 C ALA A 106 37.471 34.423 51.358 1.00 22.75 8 ATOM 847 N THR A 107 39.410 32.057 52.111 1.00 25.65 7 ATOM 848 CA THR A 107 39.410 32.057 52.111 1.00 25.65 7 ATOM 849 CB THR A 107 39.410 32.057 52.111 1.00 25.65 7 ATOM 850 OG1 THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 853 O THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 853 O THR A 107 39.706 29.637 51.713 1.00 22.75 8 ATOM 855 CG GLY A 108 43.247 31.187 53.718 1.00 28.57 6 ATOM 855 CG GLY A 108 43.247 31.187 53.718 1.00 28.57 6 ATOM 855 C GLY A 108 43.207 31.921 55.019 1.00 30.26 6 ATOM 858 N SER A 104 43.502 31.499 56.076 1.00 32.98 8 | | -21. 11 104 | 40.364 32 080 47 410 4 T | |
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| ATOM 834 N LEU A 105 41.909 33.705 48.986 1.00 25.57 6 ATOM 835 CA LEU A 105 42.163 34.698 50.008 1.00 23.91 7 ATOM 836 CB LEU A 105 42.163 34.698 50.008 1.00 23.91 7 ATOM 837 CG LEU A 105 42.049 36.082 49.382 1.00 23.57 6 ATOM 838 CD1 LEU A 105 44.502 36.551 49.672 1.00 26.30 6 ATOM 839 CD2 LEU A 105 42.823 38.413 48.984 1.00 27.36 6 ATOM 840 C LEU A 105 41.187 34.559 51.182 1.00 23.48 6 ATOM 841 O LEU A 105 41.187 34.559 51.182 1.00 23.48 6 ATOM 842 N ALA A 106 39.887 34.556 50.897 1.00 25.32 7 ATOM 843 CA ALA A 106 38.884 34.423 51.957 1.00 26.04 6 ATOM 845 C ALA A 106 37.471 34.423 51.358 1.00 24.28 6 ATOM 846 O ALA A 106 38.884 34.423 51.957 1.00 25.76 6 ATOM 847 N THR A 107 39.620 30.760 52.754 1.00 25.76 6 ATOM 848 CA THR A 107 39.620 30.760 52.754 1.00 25.54 6 ATOM 850 OG1 THR A 107 39.620 30.760 52.754 1.00 25.54 6 ATOM 851 CG2 THR A 107 39.706 29.637 51.713 1.00 21.92 6 ATOM 852 C THR A 107 39.706 29.637 51.713 1.00 21.92 6 ATOM 854 N GLY A 108 41.994 31.191 52.996 1.00 28.57 8 ATOM 855 CA GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 855 C GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 858 N SER A 109 | | 832 C SER A 104 | 41 970 32.044 45.804 1.00 35.04 | |
| ATOM 835 CA LEU A 105 | | - 55K W 103 | 42 026 33.226 1.00 25.57 | 6 |
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| ATOM 853 O THR A 107 40.901 30.720 53.583 1.00 28.16 6 ATOM 854 N GLY A 108 41.994 31.191 52.996 1.00 28.07 8 ATOM 855 CA GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 857 O GLY A 108 43.027 31.921 55.019 1.00 30.26 6 ATOM 858 N SER A 109 43.502 31.499 56.076 1.00 32.98 8 | | 851 CG2 THR A 107 | 30 340 30.000 1.00 26.40 | |
| ATOM 854 N GLY A 108 41.994 31.191 52.996 1.00 28.07 8 ATOM 855 CA GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 857 O GLY A 108 43.027 31.921 55.019 1.00 30.26 6 ATOM 858 N SER A 109 43.502 31.499 56.076 1.00 32.98 8 | | | 40.901 30.720 53.583 1.00 30.16 | |
| ATOM 855 CA GLY A 108 41.994 31.191 52.996 1.00 28.51 7 ATOM 856 C GLY A 108 43.247 31.187 53.718 1.00 28.37 6 ATOM 857 O GLY A 108 43.027 31.921 55.019 1.00 30.26 6 ATOM 858 N SER A 109 43.502 31.499 56.076 1.00 32.98 8 | | | 40.906 30.254 54.727 1.00 20.10 | |
| ATOM 856 C GLY A 108 43.027 31.187 53.718 1.00 28.37 6 ATOM 857 O GLY A 108 43.502 31.499 56.076 1.00 30.26 6 ATOM 858 N SER A 109 43.502 31.499 56.076 1.00 32.98 8 | | | 41.994 31.191 52.996 1.00 28 51 | |
| ATOM 857 O GLY A 108 43.502 31.921 55.019 1.00 30.26 6 ATOM 858 N SER A 109 43.502 31.499 56.076 1.00 32.98 8 | | | 47.000 31.18/ 53.718 1.00 28.37 | |
| ATOM 858 N SER A 109 43 331.499 56.076 1.00 32.98 8 | | 857 O GLY A 108 | 43.027 31.921 55.019 1.00 30.26 | |
| 33.018 54.942 1.00 24.81 7 | | 858 N SER A 109 | 42 322 31.499 56.076 1.00 32 98 | |
| | • | • | 33.010 34.942 1.00 24.81 | 7 |

Figure 17-14

| ATOM | 859 | CA SER A 1 | 09 | 42.002 | 33.810 | 56.119 | 1.00 24.86 | 6 |
|-------|-----|-------------|-----|--------|--------|--------|------------|-----|
| ATOM | 860 | CB SER A 1 | | 41.222 | 35.066 | 55.727 | 1.00 24.74 | 6 |
| | | _ | | | | | | |
| ATOM | 861 | OG SER A 1 | | 41.992 | 35.898 | 54.872 | 1.00 21.07 | 8 |
| ATOM | 862 | C SER A 1 | .09 | 41.240 | 32.996 | 57.173 | 1.00 27.89 | 6 |
| MOTA | 863 | O SER A 1 | .09 | 41.424 | 33.214 | 58.377 | 1.00 30.92 | 8 |
| ATOM | 864 | N THRA 1 | | 40.389 | 32.064 | 56.744 | 1.00 23.91 | 7 |
| | | | | | | 57.721 | 1.00 24.80 | 6 |
| ATOM | 865 | • | | 39.676 | 31.259 | | | |
| MOTA | 866 | CB THRA 1 | .10 | 38.641 | 30.290 | 57.074 | 1.00 29.65 | 6 |
| ATOM | 867 | OG1 THR A 1 | .10 | 37.469 | 31.016 | 56.669 | 1.00 30.45 | 8 |
| ATOM | 868 | CG2 THR A 1 | 10 | 38.228 | 29.205 | 58.067 | 1.00 29.00 | 6 |
| | 869 | C THRA 1 | | 40.712 | 30.449 | 58.478 | 1.00 24.34 | 6 |
| ATOM | | _ | | | | | | |
| MOTA | 870 | O THRA1 | | 40.615 | 30.282 | 59.699 | 1.00 24.74 | 8 . |
| ATOM | 871 | N VAL A 1 | .11 | 41.715 | 29.954 | 57.764 | 1.00 23.01 | 7 |
| ATOM | 872 | CA VAL A 1 | :11 | 42.759 | 29.173 | 58.416 | 1.00 24.13 | 6 |
| MOTA | 873 | CB VAL A 1 | 11 | 43.695 | 28.495 | 57.391 | 1.00 25.77 | 6 |
| ATOM | 874 | CG1 VAL A 1 | | 44.845 | 27.773 | 58.121 | 1.00 22.51 | 6 |
| | | | | | | | | |
| ATOM | 875 | CG2 VAL A 1 | | 42.888 | 27.502 | 56.534 | 1.00 22.67 | 6 |
| MOTA | 876 | C VAL A 1 | .11 | 43.576 | 30.071 | 59.329 | 1.00 23.14 | 6 |
| MOTA | 877 | O VAL A 1 | .11 | 43.720 | 29.793 | 60.518 | 1.00 24.11 | 8 |
| ATOM | 878 | N GLN A 1 | 12 | 44.101 | 31.156 | 58.772 | 1.00 24.94 | 7 |
| ATOM | 879 | CA GLN A 1 | | 44.895 | 32.100 | 59.554 | 1.00 25.12 | 6 |
| | | | | 45.082 | 33.413 | 58.779 | 1.00 25.14 | 6 |
| ATOM | 880 | | | | | | | |
| ATOM | 881 | CG GLN A 1 | | 45.545 | 33.224 | 57.330 | 1.00 28.51 | 6 |
| MOTA | 882 | CD GLN A 1 | .12 | 45.789 | 34.534 | 56.594 | 1.00 29.13 | 6 |
| ATOM | 883 | OE1 GLN A 1 | .12 | 46.779 | 35.219 | 56.837 | 1.00 31.22 | 8 |
| MOTA | 884 | NE2 GLN A 1 | .12 | 44.877 | 34.890 | 55.694 | 1.00 29.31 | 7 |
| ATOM | 885 | C GLN A 1 | | 44.107 | 32.362 | 60.827 | 1.00.24.62 | 6 |
| | | | | | | 61.939 | 1.00 21.10 | 8 |
| MOTA | 886 | O GLN A 1 | | 44.647 | 32.311 | | | |
| ATOM | 887 | N ALA A 1 | | 42.813 | 32.622 | 60.644 | 1.00 24.41 | 7 |
| ATOM- | 888 | CA ALA A 1 | .13 | 41.914 | 32.904 | 61.751 | 1.00 23.33 | 6 |
| ATOM | 889 | CB ALA A 1 | .13 | 40.516 | 33.183 | 61.224 | 1.00 19.80 | 6 |
| ATOM | 890 | C ALA A 1 | | 41.901 | 31.733 | 62.729 | 1.00 25.34 | 6 |
| | 891 | O ALA A 1 | | 41.925 | 31.930 | 63.946 | 1.00 27.52 | 8 |
| MOTA | | | | | | | 1.00 24.39 | 7 |
| MOTA | 892 | N ILE A 1 | | 41.859 | 30.509 | 62.211 | | |
| ATOM | 893 | CA ILE A 1 | | 41.867 | 29.356 | 63.106 | 1.00 24.49 | 6 |
| ATOM | 894 | CB ILE A 1 | .14 | 41.524 | 28.042 | 62.371 | 1.00 23.46 | 6 |
| ATOM | 895 | CG2 ILE A 1 | .14 | 41.902 | 26.855 | 63.227 | 1.00 18.97 | 6 |
| ATOM | 896 | CG1 ILE A 1 | 14 | 40.030 | 28.015 | 62.034 | 1.00 21.17 | б |
| ATOM | 897 | CD1 ILE A 1 | | 39.598 | 26.791 | 61.239 | 1.00 22.51 | 6 |
| | | | | 43.230 | 29.227 | 63.757 | 1.00 24.32 | 6 |
| ATOM | 898 | | | | | | 1.00 24.74 | 8 |
| MOTA | 899 | O ILE A 1 | | 43.328 | 28.817 | 64.907 | | |
| MOTA | 900 | N GLUA 1 | | 44.280 | 29.580 | 63.019 | 1.00 26.58 | 7 |
| MOTA | 901 | CA GLU A 1 | .15 | 45.638 | 29.518 | 63.551 | 1.00 25.89 | 6 |
| ATOM | 902 | CB GLU A 1 | .15 | 46.639 | 29.992 | 62.508 | 1.00 22.63 | 6 |
| ATOM | 903 | CG GLU A 1 | | 46.554 | 29.264 | 61.192 | 1.00 20.39 | 6 |
| | 904 | CD GLU A 1 | | 17.668 | 29.670 | 60.244 | 1.00 21.39 | 6 |
| MOTA | | | | 47.848 | | | 1.00 19.60 | 8 |
| ATOM | 905 | OE1 GLU A 1 | | | 30.887 | 60.016 | | |
| ATOM | 906 | OE2 GLU A 1 | | 18.362 | 28.769 | 59.722 | 1.00 22.53 | 8 |
| ATOM | 907 | C GLU A 1 | 15 | 45.724 | 30.422 | 64.774 | 1.00 27.56 | 6 |
| ATOM | 908 | O GLU A 1 | 15 | 46.173 | 30.006 | 65.837 | 1.00 25.98 | 8 |
| ATOM | 909 | N GLU A 1 | | 45.267 | 31.660 | 64.615 | 1.00 31.19 | 7 |
| | 910 | CA GLU A 1 | | 45.282 | 32.631 | 65.705 | 1.00 35.80 | 6 |
| ATOM | | | | | | | 1.00 36.91 | 6 |
| ATOM | 911 | CB GLU A 1 | | 44.676 | 33.959 | 65.237 | | |
| MOTA | 912 | CG GLU A 1 | | 45.434 | 34.605 | 64.069 | 1.00 41.14 | 6 |
| ATOM | 913 | CD GLU A 1 | 16 | 46.872 | 34.982 | 64.420 | 1.00 43.09 | 6 , |
| ATOM | 914 | OE1 GLU A 1 | 16 | 47.072 | 35.886 | 65.267 | 1.00 43.42 | 8 |
| | 915 | CE2 GLU A 1 | | 47.802 | 34.369 | 63.849 | 1.00 41.76 | 8 |
| ATOM | | | | 44.543 | 32.131 | 66.947 | 1.00 35.11 | 6 |
| ATOM | 916 | | | | | | | 8 |
| ATOM | 917 | O GLU A 1 | | 45.054 | 32.228 | 68.061 | 1.00 37.26 | |
| MOTA | 918 | N PHE A 1 | | 43.343 | 31.598 | 66.761 | 1.00 34.30 | 7 |
| ATOM | 919 | CA PHE A 1 | 17 | 42.577 | 31.096 | 67.893 | 1.00 34.44 | 5 |
| ATOM | 920 | CB PHE A 1 | | 41.300 | 30.399 | 67.415 | 1.00 35.45 | 6 |
| | 921 | CG PHE A 1 | | 40.383 | 29.979 | 68.533 | 1.00 37.14 | 6 |
| ATOM | | | | | | 69.290 | 1.00 35.80 | 6 |
| MOTA | 922 | CD1 PHE A 1 | | 39.705 | 30.930 | | | 6 |
| ATCM | 923 | CD2 PHE A 1 | | 40.196 | 28.630 | 68.832 | 1.00 41.05 | |
| MOTA | 924 | CE1 PHE A 1 | 17 | 38.853 | 30.549 | 70.323 | 1.00 38:08 | 6 |
| | | | | | | - | | - |
| | | | | | | | | |

| | | • |
|--------|---|--|
| ATO | M 925 CE2 PHE A 117 | 20.220 |
| ATO | M 926 CZ PHE A 117 | 39.338 28.234 69.874 1.00 40.44 |
| OTA | 05 FUL X 11/ | |
| | TO THE MITTIN | 12 124 20 22 100 38.64 |
| OTA. | M 928 O PHE A 117 | 43 400 34.24 |
| ATO | M 929 N LEU A 118 | 30.136 69.898 1 00 33 54 |
| ATO | TO W 110 | 44.069 29 194 67 033 |
| _ | THE OWN THE WATTE | 44 000 00 |
| ATO | M 931 CB LEU A 118 | |
| ATO | M 932 CG LEU A 118 | 43.133 47.036 67.488 1 00 30 E0 |
| ATO | TO CO DEC A 118 | 43.900 25.297 67 030 1 00 22 |
| | CD1 DEO R 118 | 44 244 an |
| ATON | 934 CD2 LEU A 118 | 42 252 25.336 1.00 20.81 |
| ATON | 935 C LEU A 118 | 13.433 43.00% 68 757 1 00 00 |
| | and a pro v 119 | 16 316 ST |
| ATON | DEC 7. 118 | 46 000 00 1.00 34.3/ 6 |
| ATOM | 937 N LYS A 119 | 46 461 1.00 36.15 R |
| ATOM | 938 CA LYS A 119 | 10.301 23.3/4 68.843- 1 nn 3/17e ~ |
| ATOM | Cit BIS K III | 47.679 30.609 69.365 1.00 34.75 7 |
| | E DIS A 119 | 40 343 5 5 5 5 5 5 5 5 6 5 6 6 6 6 6 6 6 6 6 |
| ATOM | 940 CG LYS A 119 | 08.448 1.00 33 52 |
| ATOM | | 31.2/0 6/.100 1 nn 37 no c |
| MOTA | DID W 113 | 49.111 32.430 66 262 |
| | | 40 601 31 - 00 43.40 6 |
| ATOM | 943 NZ LYS A 119 | |
| ATOM | 944 C LYS A 119 | 33.030 64.092 1 00 51 40 7 |
| ATOM | 5 515 A 119 | *''-4'3 31.19 //) 7/15 1 00 34 |
| | - 1 DIS A 119 | 40 110 71 400 - 100 34.05 6 |
| ATOM | 946 N GLY A 120 | 4E 000 20 20 1.00 38.12 8 |
| ATOM | 947 CA GLY A 120 | 30.007 31.374 /U.869 1 00 34 15 - |
| ATOM | 11 120 | 45.431 31.927 72 094 1 00 75 |
| | 11 120 | |
| atom | 949 O GLY A 120 | 44 640 74 6 |
| MOTA | 950 N ASN A 121 | 34.072 /2.796 1.00 40 23 0 |
| MOTA | | 44.619 33.644 70.586 1.00 38 18 |
| | | 44.079 34 956 70 347 1.00 30.48 7 |
| ATOM | 952 CB ASN A 121 | 44 000 77 100 37.47 6 |
| ATOM | 953 CG ASN A 121 | 33.024 69.170 1.00 39 57 |
| ATOM | 954 OD1 ASN A 121 | 30.340 33.8/1 69 677 1 70 40 50 |
| MOTA | | 4/.078 34 938 69 926 |
| | 955 ND2 ASN A 121 | 46 727 3 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 |
| ATOM | 956 C ASN A 121 | 42 (72 2.5) 1.00 43.63 7 |
| ATOM | 957 O ASN A 121 | ****** 1 00 36 E0 6 |
| ATOM | TTT | 42.037 33.818 69.704 1.00 36.59 6 |
| | 11 A 122 | 42 002 26 66 |
| ATOM | 959 CA VAL A 122 | 40 770 25 31 31 33 53 7 |
| ATOM | 960 CB VAL A 122 | 30.720 36.166 68.976 1.00 34.77 6 |
| ATOM | | 32.001 3/.Uh4 60 000 1 66 an |
| ATOM | | 38.418 37.096 69 399 1 00 3 |
| | 962 CG2 VAL A 122 | 30 010 37,33 6 |
| MCTA | 963 C VAL A 122 | 40 707 07 |
| ATOM | 964 O VAL A 122 | 30.731 30.781 67.596 1.00 31 08 6 |
| ATOM | 965 N ALA A 123 | ******* 37.907 67.441 1 00 34 10 0 |
| ATOM | | 40.451 35 075 66 500 |
| | 966 CA ALA A 123 | 10 15: 1 |
| ATOM | 967 CB ALA A 123 | 41 707 75 75 75 75 75 75 75 75 75 75 75 75 75 |
| ATOM | 968 C ALA A 123 | **·30/ 35.588 64.327 7 00 32 14 E |
| ATOM | | 33.030 30.533 64.716 1 00 20 20 |
| | | 20 120 |
| ATOM | 970 N PHE A 124 | 20 075 2 2 2 2 2 2 2 2 3 |
| ATOM | 971 CA PHE A 124 | 1.00 28 70 7 |
| ATOM | 972 CB PHE A 124 | 37.001 37.475. 62.976 1.00 28 39 6 |
| ATOM | 124 | 76 020 20 |
| | 973 CG PHE A 124 | 3E CAE 34 |
| ATOM | 974 CD1 PHE A 124 . | 34 670 30 31.20 6 |
| ATOM | 975 CD2 PHE A 124 | 34.079 38.139 62.564 1 00 32 00 6 |
| ATOM | 976 CE1 PHE A 124 | 35.378 40 435 62 570 |
| | | 32 463 75 100 49.33 6 |
| ATOM | 977 CE2 PHE A 124 | 24 166 40 30.74 6 |
| ATOM | . 978 CZ PHE A 124 | 40.813 61.988 1.00 27 45 6 |
| ATOM | | 33.207 39.847 61.686 1.00 39 73 6 |
| | | 37.880 37 671 61 400 |
| ATOM | 980 O PHE A 124 | 20 422 22 22 22 22 20 20 30 19 6 |
| ATOM | 981 N ASN A 125 | 33.545 36.695 61.095 1.00 32.10 8 |
| ATCM | | 2,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| | *************************************** | |
| ATOM | 983 CB ASN A 125 | 20 242 2 1.00 30.10 6 |
| ATOM | 984 CG ASN A 125 | 70 701 = 1.00 32.02 6 |
| ATOM | 985 OD1 ASN A 125 | 30.201 33.360 57.195 1.00 33 79 6 |
| | 000 ND2 ASN A 125 | 38.754 36 306 56 556 |
| ATOM | 986 ND2 ASN A 125 | |
| ATOM | 987 C ASN A 125 | |
| ATOM - | 988 O ASN A 125 | 30.403 37.083 58.584 1.00 29.80 6 |
| MOTA | | |
| | 11.0 11 120 | 7/ 17/ 2/1/24 0 |
| ATCM | 990 CD PRO A 126 | 25.300 30.431 1.00 28.25 |
| | | 36.997 39.516 58.833 1.00 29.22 6 |
| | • | |

83/263 Figure 17-16

| | | | | | | | | _ |
|--------|--------|-------|-------------|--------|----------|----------|--------------|-----|
| | 001 | CA | PRO A 126 | 34.909 | 38.891 | 57.844 | 1.00 27.92 | 6 |
| MOTA | 991 | CA | PRO A 120 | 35.139 | 40.407 | 57.856 | 1.00 29.07 | 6 |
| MOTA | 992 | CB | PRO A 126 | | | 57.775 | 1.00 26.54 | 6 |
| MOTA | 993 | CG | PRO A 126 | 36.649 | 40.520 | | | |
| | 994 | С | PRO A 126 | 34.651 | 38.339 | 56.448 | 1.00 27.54 | 6 |
| MOTA | | ō | PRO A 126 | 33.532 | 38.402 | 55.949 | 1.00 28.66 | 8 |
| ATOM | 995 | | | 35.687 | 37.795 | 55.820 | 1.00 26.99 | 7 |
| ATOM | 996 | N | ALA A 127 | | | | 1.00 26.54 | 6 |
| ATOM | 997 | CA | ALA A 127 | 35.548 | 37.244 | 54.477 | | |
| | 998 | СВ | ALA A 127 | 36.822 | 37.505 | 53.684 | 1.00 22.43 | 6 |
| ATOM | | | | 35.225 | 35.744 | 54.480 | 1.00 27.38 | 6 |
| MOTA | 999 | С | ALA A·127 | | 35.140 | 53.423 | 1.00 29.04 | 8 |
| ATOM | 1000 | 0 | ALA A 127 | 35.038 | | | 1.00 25.04 | 7 |
| MOTA | 1001 | N | GLY A 128 | 35.166 | 35.142 | 55.663 | 1.00 26.97 | |
| | 1002 | CA | GLY A 128 | 34.874 | 33.724 | 55.737 | 1.00 25.65 | 6 |
| MOTA | | | | 33.389 | 33.486 | 55.880 | 1.00 26.17 | 6 |
| MOTA | 1003 | С | GLY A 128 | | 34.428 | 55.804 | 1.00 27.39 | 8 |
| ATOM. | 1004 | 0 | GLY A 128 | 32.600 | | | | 7 |
| ATOM | 1005 | N | GLY A 129 | 32.998 | 32.234 | 56.083 | | |
| | 1006 | CA | GLY A 129 | 31.588 | 31.936 | 56.236 | 1.00 25.17 | 6 |
| MOTA | | | GLY A 129 | 30.847 | 31.674 | 54.937 | 1.00 25.88 | 6 |
| MOTA | 1007 | С | | | 31.908 | 54.848 | 1.00 25.07 | 8 |
| MOTA | 1008 | 0 | GLY A 129 | 29:643 | | | 1.00 25.69 | 7 |
| MOTA | 1009 | N | MET A 130 | 31.566 | 31.198 | 53.927 | | |
| | 1010 | CA | MET A 130 | 30.981 | 30.872 | 52.622 | 1.00 26.48 | 6 |
| MOTA | | | MET A 130 | 32.103 | 30.907 | 51.567 | 1.00 28.53 | 6 |
| MOTA | 1011 | CB | | | 32.288 | 51.467 | 1.00 26.54 | 6 |
| ATOM | 1012 | CG | MET A 130 | 32.795 | | | 1.00 26.29 | 16 |
| ATOM | 1013 | SD | MET A 130 | 34.413 | 32.366 | 50.613 | | |
| | 1014 | CE | MET A 130 | 34.080 | 31.512 | 49.062 | 1.00 25.85 | 6 |
| ATOM | | | MET A 130 | 30.355 | 29.463 | 52.768 | 1.00 24.47 | 6 |
| ATOM | 1015 | C | | 30.761 | 28.502 | 52.113 | 1.00 17.67 | 8 |
| ATOM | 1016 | 0 | MET A 130 | | | 53.636 | 1.00 23.28 | 7 |
| MOTA | 1017 | N | HIS A 131 | 29.347 | 29.389 | | 1.00 25.20 | 6 |
| | 1018 | CA | HIS A 131 | 28.647 | 28.161 | 54.019 | 1.00 26.33 | |
| ATOM | 1019 | СВ | HIS A 131 | 27.685 | 28.485 | 55.180 | 1.00 26.98 | 6 |
| MOTA | | | | 26.663 | 29.540 | 54.862 | 1.00 28.50 | 6 |
| MOTA | 1020 | CG | HIS A 131 | | 30.030 | 53.677 | 1.00 28.65 | 6 |
| MOTA | 1021 | | HIS A 131 | 26.225 | | | 1.00 33.04 | 7 |
| MOTA | 1022 | ND1 | HIS A 131 | 25.906 | 30.166 | 55.831 | | |
| | 1023 | CET | HIS A 131 | 25.051 | 30.995 | 55.259 | 1.00 27.75 | 6 |
| ATOM | | - CD1 | HIS A 131 | 25.224 | 30.932 | 53.952 | 1.00 26.97 | 7 |
| MOTA | 1024 | | HIS W 131 | 27.917 | 27.284 | 53.017 | 1.00 28.44 | 6 |
| ATOM . | . 1025 | С | HIS A 131 | | | 53.390 | 1.00 31.15 | .3. |
| ATOM | 1026 | 0 | HIS A 131 | 27.434 | 26.214 | | 1.00 30.64 | 7 |
| ATOM | 1027 | N | HIS A 132 | 27.861 | 27.694 | 51.756 | | |
| | 1028 | CA | HIS A 132 | 27.111 | 26.938 | 50.746 | 1.00 28.71 | 6 |
| MOTA | | | HIS A 132 | 26.321 | 27.941 | 49.890 | 1.00 27.21 | 6 |
| MOTA | 1029 | CB | | | 28.819 | 50.693 | 1.00 28.83 | 6 |
| ATOM | 1030 | CG | HIS A 132 | 25.408 | | | 1.00 28.92 | 6 |
| ATOM | 1031 | CD2 | HIS A 132 | 25.111 | 30.137 | | | 7 |
| | 1032 | NID1 | HIS A 132 | 24.686 | 28.360 | 51.773 | 1.00 31.80 | |
| MOTA | | CEI | HIS A 132 | 23.981 | 29.353 | 52.285 | 1.00 29.95 | 6 |
| MOTA | 1033 | CEA | . HIS A 133 | 24.222 | | | 1.00 28.21 | 7 |
| ATOM | 1034 | NEZ | HIS A 132 | | | | | 6 |
| ATOM | 1035 | С | HIS A 132 | 27.889 | | | | 8 |
| ATOM | 1036 | 0 | HIS A 132 | 27.399 | . 24.375 | 49.533 | | 7 |
| | 1037 | N | ALA A 133 | 29.093 | 26.379 | 49.455 | | |
| MOTA | | | ALA A 133 | 29.958 | 25.586 | 48.579 | 1.00 26.99 | 6 |
| MOTA | 1038 | CA | WITH WITH | | | | | 6 |
| MOTA | 1039 | CB | ALA A 133 | 31.295 | | | | 6 |
| ATOM | 1040 | С | ALA A 133 | 30.199 | | | | 8 |
| | 1041 | 0 | ALA A 133 | 30.703 | 23.973 | | | |
| MOTA | | - | PHE A 134 | 29.850 | 23.174 | 48.255 | 1.00 26.73 | 7 |
| MOTA | 1042 | N | PRE A 134 | | | | | 6 |
| ATOM | 1043 | CA | PHE A 134 | 30.046 | | | | 6 |
| ATOM | 1044 | CB | PHE A 134 | 29.070 | | | | 6 |
| | 1045 | CG | PHE A 134 | 27.629 | 21.199 | | | |
| MOTA | | CD. | PHE A 134 | 26.929 | | 47.169 | | 6 |
| MOTK | 1046 | CD. | rur n 134 | | | | | 6 |
| MOTA | 1047 | CD | 2 PHE A 134 | 26.985 | | | | 6 |
| MOTA | 1048 | CE: | L PHE A 134 | 25.614 | | | | 6 |
| | 1049 | CE. | 2 PHE A 134 | 25.670 | 21.184 | | | |
| MOTA | | | PHE A 134 | 24.985 | | | 1.00 14.59 | |
| MOTA | 1050 | CZ | rne m 134 | | | | | 6 |
| ATOM | 1051 | С | PHE A 134 | 31.460 | | | | |
| ATOM | 1052 | 0 | PHE A 134 | 32.291 | | | | _ |
| | 1053 | N | LYS A 135 | 31.713 | 3 20.04 | | | • |
| ATOM | | | LYS A 135 | 33.012 | | 7 48.427 | | |
| aton | 1054 | CA | 115 K 135 | | | | 5 1.00 29.45 | |
| ATCM | 1055 | CB | LYS A 135 | 32.92 | | 1 48.63 | | _ |
| 3 TOM | 1056 | CG | LYS A 135 | 34.15 | 2 17.13 | T 30.03 | | • |

| MOTA | 1057 | 7 C | D LYS A 135 | | 33.965 | 15.734 | 49.221 | 1 00 20 67 | _ |
|--------------|--------------|----------|------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM- | 1058 | 3 C | E LYS A 135 | | 34.234 | | | | 6 6 |
| MOTA | 1059 | 9 N: | | | 35.679 | | | 1.00 26.25 | |
| MOTA | 1060 |) C | LYS A 135 | | 33.513 | | | 1.00 30.22 | 7 |
| ATOM | 1061 | L O | LYS A 135 | | 34.714 | | 46.763 | 1.00 30.00 | 6 |
| ATOM | 1062 | N 2 | SER A 136 | | 32.600 | | 46.028 | 1.00 31.69 | 8 7 |
| ATOM | 1063 | 3 C2 | A SER A 136 | | 32.995 | | 44.619 | 1.00 32.88 | |
| MOTA | 1064 | l CI | 3 SER A 136 | | 33.038 | | 44.040 | 1.00 31.41 | 6 6 |
| ATOM | 1065 | 5 00 | S SER A 136 | | 33.882 | | 44.810 | 1.00 35.41 | |
| ATOM | 1066 | C | SER A 136 | | 32.097 | | 43.727 | 1.00 33.55 | 8 |
| ATOM | 1067 | 7 0 | SER A 136 | | 31.921 | 20.031 | 42.553 | 1.00 36.11 | 6 8 |
| ATOM | 1068 | N | ARG A 137 | | 31.536 | | 44.262 | 1.00 30.61 | 7 |
| ATOM | 1069 |) CF | ARG A 137 | | 30.664 | 22.272 | 43.459 | 1.00 32.28 | 6 |
| ATOM | 1070 | CE | | | 29.324 | 21.554 | 43.202 | 1.00 35.91 | 6 |
| MOTA | 1071 | | | | 28.224 | 22.458 | 42.627 | 1.00 43.90 | 6 |
| ATOM | 1072 | |) ARG A 137 | | 26.819 | 21.836 | 42.751 | 1.00 48.28 | 6 |
| ATOM | 1073 | | | | 26.571 | 20.767 | 41.787 | 1.00 53.38 | 7 |
| ATOM | 1074 | | | | 26.150 | 20.960 | 40.538 | 1.00 55.30 | 6 |
| ATOM | 1075 | | 11 ARG A 137 | | 25.921 | 22.185 | 40.090 | 1.00 54.06 | 7 |
| MOTA | 1076 | | 2 ARG A 137 | | 25.969 | 19.922 | 39.728 | 1.00 58.96 | 7 |
| ATOM | 1077 | | ARG A 137 | | 30.405 | 23.631 | 44.113 | 1.00 30.24 | 6 |
| ATOM | 1078 | | ARG A 137 | | 30.380 | 23.748 | 45.338 | 1.00 23.11 | 8 |
| MOTA | 1079 | | ALA A 138 | | 30.219 | 24.653 | 43.279. | 1.00 27.33 | 7 |
| ATOM | 1080 | | | | 29.944 | 26.000 | 43.757 | 1.00 27.36 | 6 |
| ATOM | 1081 | CB | | | 30.149 | 26.997 | 42.645 | 1.00 27.57 | 6 |
| MOTA | 1082 | c | ALA A 138 | | 28.496 | 26.003 | 44.213 | 1.00 26.45 | 6 |
| MOTA | 1083 | 0 | ALA A 138 | | 27.747 | 25.083 | 43.865 | 1.00 27.30 | 8 |
| ATOM ATOM | 1084 1085 | N CA | ASN A 139 | | 28.090 | 27.021 | 44.975 | 1.00 22.47 | 7 |
| ATOM | 1086 | CB | | | 26.711 | 27.063 | 45.471 | 1.00 23.85 | 6 |
| ATOM | 1087 | CG | ASN A 139 | | 26.406 | 25.738 | 46.218 | 1.00 16.82 | 6 |
| ATOM | 1088 | | 1 ASN A 139 | | 25.040 24.019 | 25.718 | 46.900 | 1.00 14.45 | 6 |
| ATOM | 1089 | | 2 ASN A 139 | | 25.018 | 26.084 | 46.319 | 1.00 13.39 | 8 |
| MOTA | 1090 | C | ASN A 139 · | | 26.444 | 25.249 28.277 | 48.139 | 1.00 20.08 | 7 |
| ATOM | 1091 | ō | ASN A 139 | | 27.239 | 28.600 | 46.368 47.260 | 1.00 26.09 | 6 |
| MOTA | 1092 | N | GLY A 140 | | 25.326 | 28.954 | 46.114 | 1.00 27.50 | 8 |
| ATOM | 1093 | CA | GLY A 140 | | 24.965 | 30.106 | 46.916 | 1.00 24.83 1.00 22.24 | 7 |
| ATOM | 1094 | С | GLY A 140 | | 25.991 | 31.211 | 46.890 | 1.00 22.24 | 6 6 |
| MOTA | 1095 | 0 | GLY A 140 | | 26.256 | | 47.910 | 1.00 23.50 | 8 |
| ATOM | 1096 | N | PHE A 141 | | 26.570 | 31.437 | 45.717 | 1.00 25.60 | 7 |
| MOTA | 1097 | CA | PHE A 141 | | 27.582 | 32.476 | 45.518 | 1.00 26.47 | 6 |
| MOTA | 1098 | CB | PHE A 141 | | 27.204 | 33.765 | 46.258 | 1.00 28.05 | 6 |
| ATOM | 1099 | CG | PHE A 141 | | 25.925 | 34.391 | 45.792 | 1.00 28.61 | 6 |
| MOTA | 1100 | | PHE A 141 | | 25.352 | 35.428 | 46.518 | 1.00 30.74 | 6 |
| ATOM | 1101 | CD2 | | | 25.312 | 33.975 | 44.620 | 1.00 29.10 | 6 |
| MG A | 1102 | | PHE A 141 | | 24.193 | 36.044 | 46.087 | 1.00 29.33 | 6 |
| A L'OM | 1103 | | PHE A 141 | - | 24.150 | 34.583 | 44.177 | 1.00 31.03 | 6 |
| ATCM | 1104 1105 | CZ | PHE A 141 | | 23.589 | 35.621 | 44.912 | 1.00 32.59 | 6 |
| ATOM | 1105 | .c | PHE A 141 | | 28.954 | 32.038 | 45.991 | 1.00 24.63 | 6 |
| MOTA MOTA | 1100 | O | PHE A 141 | | 29.938 | 32.727 | 45.733 | 1.00 29.72 | 8 |
| ATOM | 1107 | N | CYS A 142 | | 29.025 | | 46.667 | 1.00 21.11 | 7. |
| ATOM | 1108 | CA CB | CYS A 142 CYS A 142 | | 30.296 | 30.399 | 47.192 | 1.00 22.30 | 6 |
| ATOM | 1110 | SG | CYS A 142 | | 30.062 | 29.787 | 48.567 | 1.00 21.31 | 6 |
| MOTA | 1111 | C | | | 28.943 | 30.748 | 49.582 | 1.00 22.93 | 16 |
| ATOM | 1112 | 0 | CYS A 142 CYS A 142 | | 31.017 | 29.366 | 46.326 | 1.00 22.13 | 6 |
| ATOM | 1113 | Ŋ | TYR A 143 | | 30.408 32.317 | 28.389 29.573 | 45.878 | 1.00 22.97 | 8 |
| ATOM | 1114 | CA | TYR A 143 | | 33.129 | 43.5/3 | 46.111 | 1.00 23.09 | 7 |
| MOTA | 1115 | CB | TYR A 143 | | 34.063 | 28.632 | 45.335 | 1.00 23.05 | 6 |
| ATOM | 1116 | CG | TYR A 143 | | 33.377 | 29.365 30.379 | 44.375 | 1.00 21.60 | 6 |
| ATOM | 1117 | | TYR A 143 | | 32.969 | 31.609 | 43.487 | 1.00 24.09 | 6 |
| ATOM | 1118 | | TYR A 143 | | 32.365 | 32.555 | 43.999 43.199 | 1.00 23.29 1.00 23.26 | 6 |
| ATOM | 1119 | | TYR A 143 | | 33.154 | 30.117 | 43.139 | 1.00 23.26 | 6. |
| ATOM | 1120 | | TYR A 143 | | 32.544 | 31.061 | 42.133 | 1.00 24.82 | 6 6 |
| ATOM | 1121 | CZ | TYR A 143 | | 32.153 | 32.281 | 41.857 | 1.00 24.82 | 6 |
| ATOM | 1122 | OH | TYR A 143 | | 31.553 | 33.241 | 41.064 | 1.00 32.35 | 8 |
| | - | | | | | 531 | | 2.00 32.33 | J |

| | - 1 2 2 | С | TYR A 143 | | 33.960 | 27 | .766 | 46.290 | 1.00 24.22 | | |
|--------------|--------------|----------|------------------------|---|------------------|-----|----------------|--------------------|------------|----------------|---|
| MOTA | 1123 | 0 | TYR A 143 | | 34.266 | 26 | .606 | 45.998 | 1.00 24.58 | | |
| ATOM | 1124 | N | ILE A 144 | | 34.327 | 28 | .329 | 47.437 | 1.00 23.83 | | |
| MOTA | 1125 | CA | ILE A 144 | | 35.086 | 27 | .566 | 48.425 | 1.00 20.24 | | |
| MOTA | 1126 | CB | ILE A 144 | | 36.547 | 27 | .982 | 48.453 | 1.00 17.27 | | |
| MOTA | 1127 | CG2 | | | 37.231 | 27 | .354 | 49.662 | 1.00 11.03 | | |
| MOTA | 1128 | CGZ | ILE A 144 | | 37.185 | 27 | .603 | 47.110 | 1.00 14.93 | | |
| MOTA | 1129 | | | | 38.601 | | .028 | 46.946 | 1.00 19.68 | | |
| ATOM | 1130 | CD1 | ILE A 144 | | 34.495 | 27 | .703 | 49.815 | 1.00 21.77 | | |
| MOTA | 1131 | C | ILE A 144 | | 34.288 | | .811 | 50.318 | 1.00 21.19 | | |
| ATOM | 1132 | 0 | ASN A 145 | _ | 34.212 | 26 | . 555 | 50.424 | 1.00 23.00 | | |
| MOTA | 1133 | N | ASN A 145 | | 33.616 | 26 | .508 | 51.750 | 1.00 20.92 | | • |
| ATOM | 1134 | CA | ASN A 145 | | 32.902 | 2.5 | .170 | 51.935 | 1.00 17.0 | | |
| MOTA | 1135 | CB CG | ASN A 145. | | 32.079 | 25 | .125 | 53.203 | 1.00 21.0 | | |
| MOTA | 1136 | | ASN A 145 | | 32.549 | | .508 | 54.276 | 1.00 20.9 | | |
| MOTA | 1137 | ND2 | | | 30.844 | 24 | .640 | 53.093 | 1.00 20.9 | | |
| MOTA | 1138 | C | ASN A 145 | | 34.706 | 26 | 6.669 | 52.806 | 1.00 19.6 | | |
| MOTA | 1139 1140 | ò | ASN A 145 | | 35.201 | 25 | 6.679 | 53.351 | 1.00 20.6 | | |
| MOTA | | N | ASN A 146 | | 35.079 | 27 | 7.911 | 53.100 | 1.00 16.2 | | |
| MOTA | 1141 1142 | CA | ASN A 146 | | 36.123 | | 3.143 | 54.088 | 1.00 19.3 | | |
| MOTA | 1143 | CB | ASN A 146 | | 36.428 | | 651 | 54.207 | 1.00 20.2 | | |
| MOTA | 1144 | CG | ASN A 146 | | 35.292 | 30 | 0.444 | 54.795 | 1.00 18.0 | | |
| MOTA | 1145 | 001 | ASN A 146 | | 35.079 | | 0.421 | 55.999 | 1.00 25.8 | | |
| MOTA | 1146 | | ASN A 146 | | 34.552 | | 1.149 | 53.948 | 1.00 16.0 | | |
| ATOM | 1147 | С | ASN A 146 | | 35.775 | | 7.504 | 55.443 | 1.00 20.4 | - | |
| MOTA | 1148 | ō | ASN A 146 | | 36.663 | | 7.027 | 56.151 | 1.00 19.8 | | |
| ATOM | 1149 | N | PRO A 147 | | 34.482 | | 7.485 | 55.819 | 1.00 19.3 | | |
| MOTA MOTA | 1150 | CD | PRO A 147 | | 33.312 | _ | 8.068 | 55.135 | 1.00 17.4 | | |
| ATOM | 1151 | CA | PRO A 147 | | 34.058 | | 6.877 | 57.087 | 1.00 22.2 | | |
| ATOM | 1152 | CB | PRO A 147 | | 32.539 | | 7.065 | 57.057 | 1.00 20.8 | _ | |
| MOTA | 1153 | CG | PRO-A 147 | | 32.407 | | 8.378 | 56.305 | 1.00 26.8 | - | |
| ATOM | 1154 | С | PRO A 147 | | 34.443 | _ | 5.383 | 57.188 58.169 | 1.00 29.1 | | |
| ATOM | 1155 | 0 | PRO A 147 | | 35.066 | _ | 4.954. | 56.176 | 1.00 25.8 | _ | |
| ATOM | 1156 | N | ALA A 148 | | 34.070 | _ | 4.596 3.164 | 56.174 | 1.00 25.4 | | |
| ATOM | 1157 | CA | ALA A 148 | | 34.372 | _ | 2.468 | 55.009 | 1.00 21. | | |
| ATOM | 1158 | CB | ALA A 148 | | 33.670 35.870 | _ | 2.916 | 56.100 | 1.00 25. | 94 6 | |
| MOTA | 1159 | С | ALA A 148 | | 36.382 | _ | 1.971 | 56.701 | 1.00 27. | | |
| ATOM | 1160 | 0 | ALA A 148 | | 36.574 | | 3.756 | 55.349 | 1.00 26. | | |
| MOTA | 1161 | N | VAL A 149 | | 38.017 | | 3.609 | 55.233 | 1.00 24. | | |
| MOTA | 1162 | CA | VAL A 149 VAL A 149 | | 38.622 | _ | 4.663 | 54.267 | 1.00 26. | | |
| MOTA | 1163 | CB | 1 VAL A 149 | | 40.135 | _ | 4.476 | 54.158 | 1.00 25. | | |
| MOTA | 1164 | | | | 37.970 | | 24.544 | | 1.00 26. | | |
| MOTA | 1165 | | VAL A 149 | | 38.51 | | 23.870 | | 1.00 23. | | |
| MOTA | 1166 | | VAL A 149 | | 39.45 | | 23.228 | | 1.00 19. | | |
| MOTA | 1167 | | GLY A 150 | | 37.85 | | 24.815 | 57,299 | | | |
| MOTA | 1168 | | | | 38.21 | 0 2 | 25.175 | | | | |
| ATOM | 1169 1170 | | GLY A 150 | | 38.13 | Ò : | 23.975 | 59.568 | | 19 6 | |
| ATOM | 1171 | | GLY A 150 | | 39.11 | | 23.620 | | | .05 8 .56 7 | |
| MOTA | 1172 | | ILE A 151 | | 36.95 | | 23.348 | | | | |
| MOTA | 1173 | | | | 36.77 | | 22.176 | 60.457 | | | |
| ATOM | 1174 | | | | 35.31 | | 21.654 | 60.389 | 1.00 29 | .02 6 | |
| ATOM | | | | | 35.25 | | 20.215 | | | .31 6 | |
| MOTA | | | 1 ILE A 151 | | 34.39 | | 22.540 | | | .83 | |
| MOTA | | | 1 ILE A 151 | | 34.25 | - | 23.967 | | | | |
| MOTA | 4450 | | ILE A 151 | | 37.72 | | 21.039 | | | | |
| MOTA | | _ | ILE A 151 | | 38.34 | | 20.420 | | | _ | |
| MOTA | 4400 | | GLU A 152 | | 37.84 | | 20.769 | | | | 6 |
| MOTA MOTA | | | GLU A 152 | | 38.70 | | 19.69 | | | | 6 |
| ATOM | · | | GLU A 152 | | 38.57 | | 19.52 | | | | 6 |
| | | | GLU A 152 | | 37.26 | | 18.84 | | | | 6 |
| atom atom | | CI | GLU A 152 | | 37.12 | | 17.44 | | | | 8 |
| atom atom | | 5 01 | 21 GLU A 152 | | 36.08 | | 16.77 | 9 56.71 2 57.72 | | | 8 |
| | • ••• | | 22 GLU A 152 | | 38.03 | | 16.99 | | | | 6 |
| ATOM TOM | | | GLU A 152 | | 40.14 | | 19.90 | | | | 8 |
| ATOM | • ••• | | GLU A 152 | | 40.87 | 79 | 18.94 | 6 58.97 | o 1.00 J0 | | - |
| | | | | | | | | | | | |

| ATOM | 1189 N TYR A 153 | 40.541 21.170 58 765 1 00 22 00 | |
|------|---------------------|--|----|
| ATOM | 1190 CA TYR A 153 | 41 005 | 7 |
| MCTA | 33 | 41.0/3 21.563 59.193 1.00 32.04 | 6 |
| ATOM | | 42.019 23.074 59.058 1.00 34.88 | 6 |
| ATOM | | 43.280 23.667 59.639 1.00 38 03 | 6 |
| ATOM | | 44 498 22 611 50 040 | |
| | | 45 658 24 207. E0 47E 4 55 | 6 |
| ATCM | | 43 250 24 321 60 260 | 6 |
| MCTA | 1196 CE2 TYR A 153 | 44 307 | 6 |
| ATOM | 1197 CZ TYR A 153 | 45 500 | 6 |
| ATOM | 1198 OH TYR A 153 | 3.367 24.860 60.704 1.00 43 34 | б |
| ATOM | 1199 C TYR A 153 | 40.096 25.480 61.241 1.00 44.86 | 8 |
| ATOM | 233 | 41.919 21.168 60.667 1.00 32 50 | 6 |
| | 255 | 44.00/ 20 518 67 120 1 60 55 5 | |
| ATOM | | 40 969 21 550 61-32 | В |
| MOTA | 1202 CA LEU A 154 | 40 730 21 261 62 222 | 7 |
| MOTA | 1203 CB LEU A 154 | 30 442 04.525 1.00 49.38 | 6 |
| ATOM | 1204 CG LEU A 154 | | 5 |
| MOTA | 1205 CD1 LEU A 154 | 23 001 21.00 31.20 | 5. |
| ATOM | 1206 CD2 LEU A 154 | 40 440 66 | 5 |
| ATOM | 1207 C LEU A 154 | 40.418 23.787 64.691 1.00 24.95 | |
| MCTA | | 40.732 19.772 63.146 1.00 29 56 | |
| | 252 | 41.223 10 363 64 106 1 1 | |
| ATOM | 1209 N ARG A 155 | 40 174 19 050 63 055 | |
| ATOM | 1210 CA ARG A 155 | 40 124 | |
| ATOM | 1211 CB ARG A 155 | 20 10 | i |
| ATOM | 1212 CG ARG A 155 | 32 200 | j |
| ATOM | 1213 CD ARG A 155 | 25 572 | ; |
| MOTA | 1214 NE ARG A 155 | 36.678 16.719 60.863 1.00 32.92 6 | i |
| ATOM | 1215 CZ ARG A 155 | 36.152 15.451 61.363 1.00 33.98 7 | |
| ATOM | | 33.195 14.760 60.741 1.00 37 93 6 | |
| ATOM | | 34.0/1 15.216 59.605 1.00 38 30 7 | |
| | 1217 NH2 ARG A 155 | 34 732 12 631 61 200 | |
| ATOM | 1218 C ARG A 155 | 41 521 16 920 62 221 | |
| ATOM | 1219 O ARG A 155 | 1,00 33,97 6 | |
| ATOM | 1220 N LYS A 156 | 42 319 17 540 63 1.00 32.95 8 | |
| ATOM | 1221 CA LYS A 156 | 43 679 17 001 51 1.00 34.20 7 | |
| ATOM | 1222 CB LYS A 156 | 14 212 | |
| ATOM | 1223 CG LYS A 156 | 12 11 11 11 11 11 11 11 11 11 11 11 11 1 | |
| ATOM | 1224 CD LYS A 156 | 43.0/3 17.187 59.638 1.00 40 32 6 | |
| ATOM | | 46.116 17.532 58.220 1.00 40.33 6 | |
| ATOM | 250 | 45.180 16.909 57.184 1.00 41 27 6 | |
| | | 45.015 15.435 57.364 1.00 37.92 7 | |
| MCTA | 1227 C LYS A 156 | 44 539 17 501 62 400 | |
| MCTA | 1228 O LYS A 156 | 45 582 16 905 62 622 | |
| MCTA | 1229 N LYS A 157 | 44 093 19 537 63 130 1.00 34.53 8 | |
| MOTA | 1230 CA LYS A 157 | 44 820 19 026 64 204 | |
| MOTA | 1231 CB LYS A 157 | 44 495 20 501 64 566 1.00 37.09 6 | |
| MCTA | 1232 CG LYS A 157 | 44 000 | |
| MCTA | 1233 CD LYS A 157 | 46 460 30.22 6 | |
| MOTA | 1234 · TE LYS A 157 | 46.468 21.231 63.239 1.00 37.91 6 | |
| ATOM | 1235 JZ LYS A 157 | 46.993 22.100 62.107 1.00 39.35 6 | |
| ATOM | | 48.434 21.815 61.842 1.00 38 70. 7 | |
| | | 44.498 18.178 65.515 1.00 35.61 6 | |
| ATOM | 1237 O LYS A 157 | 45.204 18.232 66.518 1.00 36.38 8 | |
| ATCM | 1238 N GLY A 158 | 43.433 17.392 65 431 1 00 34 37 7 | |
| MOTA | 1239 CA GLY A 158 | | |
| ATCM | 1240 C GLY A 158 | | |
| ATCM | 1241 O GLY A 158 | 44 1.00 30.78 6 | |
| ATOM | 1242 N PHE A 159 | 8 41.07 | |
| MOTA | 1243 CA PHE A 159 | 41.023 17.791 66.855 1.00 36.75 7 | |
| ATOM | 1244 CB PHE A 159 | 39.743 18.046 67.505 1.00 33.83 6 | |
| | | 39.246 19.459 67.213 1.00 32.65 6 | |
| MOTA | | 40.115 20.521 67.787 1.00 29.97 6 | |
| ATOM | 1246 CD1 PHE A 159 | 41.404 20.724 67 297 1 00 30 30 | |
| MCTA | 1247 CD2 PHE A 159 | 39 672 21 200 60 252 | |
| MCTA | 1248 CE1 PHE A 159 | | |
| MOTA | 1249 CE2 PHE A 159 | 10 409 22 246 | |
| ATCM | 1250 CZ PHE A 159 | 3,420 4,00 23,87 3 | |
| ATOM | 1251 C PHE A 159 | | |
| ATCM | | 38.732 17.026 67.025 1.00 33.41 6 | |
| | | 38.664 16.716 65.838 1.00 31.61 8 | |
| ATCH | | 37.951 16.506 67.966 1.00 35.13 7 | |
| MOTA | 1254 CA LYS A 160 | 36:947 15.493 67.677 1.00 35.39 6 | |
| | | - 10,7 - 10,33,39 6 | |

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| ATOM | 1255 | CB | LYS | A 160 | 37.342 | 14.198 | 68.389 | 1.00 36.43 | 6 |
|------|-------|-----|-------|--------|----------|--------|------------------|--------------------------|--------|
| ATOM | 1256 | CG | LYS | A 160 | 38.535 | 13.502 | 67.708 | 1.00 40.67 | 6 |
| ATOM | 1257 | CD | | A 160 | 39.312 | 12.538 | 68.615 | 1.00 44.68 | 6 |
| | 1258 | CE | | A 160 | 38.425 | 11.536 | 69.345 | 1.00 49.23 | 6 |
| ATOM | 1259 | NZ | | A 160 | 37.593 | 12.182 | 70.411 | 1.00 50.63 | 7 |
| ATOM | 1260 | | | A 160 | 35.524 | 15.927 | 68.027 | 1.00 35.94 | 6 |
| MOTA | | C. | | | 34.561 | 15.241 | 67.691 | 1.00 35.72 | 8 |
| MOTA | 1261 | - | - | A 160 | | | 68.718 | 1.00 34.35 | 7 |
| ATOM | 1262 | N | | A 161 | 35.399 | 17.058 | | | |
| ATOM | 1263 | CA | | A 161 | 34.091 | 17.618 | 69.044 | 1.00 34.95 | 6 |
| ATOM | 1264 | CB | | A 161 | 33.771 | 17.525 | 70.535 | 1.00 33.94 | 6 |
| MOTA | 1265 | CG | | A 161 | . 33.427 | 16.132 | 70.992 | 1.00 38.25 | 6 |
| MOTA | 1266 | CD | ARG | A 161 | 32.823 | 16.131 | 72.386 | 1.00 41.17 | 6. |
| ATOM | 1267 | NE | ARG . | A 161 | 33.719 | 16.722 | 73.378 | 1.00 47.64 | 7 |
| ATOM | 1268 | CZ | ARG . | A 161 | 34.912 | 16.233 | 73.705 | 1.00 47.92 | 6 |
| ATOM | 1269 | NH1 | ARG . | A 161 | 35.372 | 15.131 | 73.121 | 1.00 47.56 | 7 |
| ATOM | 1270 | NH2 | ARG . | A 161 | 35.648 | 16.858 | 74.615 | 1.00 46.95 | 7 |
| ATOM | 1271 | С | ARG . | A 161 | 34.113 | 19.076 | 68.598 | 1.00 34.58 | 6 |
| ATOM | 1272 | 0 | ARG . | A 161 | 34.468 | 19.980 | 69.357 | 1.00 33.77 | 8 |
| ATOM | 1273 | N | ILE . | A 162 | 33.741 | 19.280 | 67.341 | 1.00 31.74 | 7 |
| ATOM | 1274 | CA | ILE . | A 162 | 33.735 | 20.594 | 66.735 | 1.00 29.83 | 6 |
| ATOM | 1275 | CB | ILE . | A 162 | 34.429 | 20.542 | 65.362 | 1.00 29.96 | 6 |
| ATOM | 1276 | CG2 | ILE . | A 162 | 34.580 | 21.942 | 64.784 | 1.00 30.57 | 6 |
| ATOM | 1277 | CG1 | ILE . | A 162 | 35.801 | 19.891 | 65.522 | 1.00 28.81 | 6 |
| ATOM | 1278 | | | A 162 | 36.537 | 19.685 | 64.224 | 1.00 33.05 | 6 |
| ATOM | 1279 | c | | A 162 | 32.300 | 21.050 | 66.560 | 1.00 29.66 | 6 |
| ATOM | 1280 | ō | | A 162 | 31.416 | 20.241 | 66.266 | 1.00 25.24 | 8 |
| ATOM | 1281 | N | | A 163 | 32.081 | 22.351 | 66.745 | 1.00 30.00 | 7 |
| MOTA | 1282 | CA | | A 163 | . 30.754 | 22.945 | 66.617 | 1.00 30.48 | б |
| ATOM | 1283 | CB | LEU . | A 163 | 30.236 | 23.406 | 67.992 | 1.00 32.25 | 6 |
| ATOM | 1284 | CG | LEU . | A 163 | 28.934 | 24.229 | 68.044 | 1.00 31.21 | 6 |
| ATOM | 1285 | CD1 | LEU . | A 163 | 27.804 | 23.494 | 67.326 | 1.00 31.58 | 6 |
| ATOM | 1286 | CD2 | LEU . | A 163 | 28.569 | 24.502 | 69.493 | 1.00 25.00 | Ġ |
| ATOM | 1287 | С | LEU . | A 163 | 30.717 | 24.122 | 65.659 | 1.00 29.23 | 6 |
| ATOM | 1288 | ,0 | LEU . | A 163 | 31.596 | 24.980 | 65.654 | 1.00 29.72 | 8 |
| ATOM | 1289 | N | TYR . | A 164 | 29.675 | 24.157 | 64.846 | 1.00 29.68 | 7 |
| ATOM | 1290 | CA | TYR . | A 164 | 29.500 | 25.244 | 63.899 | 1.00 29.89 | 6 |
| ATOM | 1291 | CB | TYR . | A 164 | 29.512 | 24.688 | 62.470 | 1.00 27.81 | 6 |
| ATOM | 1292 | CG | TYR . | A 164 | 29.377 | 25.742 | 61.399 | 1.00 27.79 | 6 |
| MOTA | 1293 | | | A 164 | 30.390 | 26.670 | 61.168 | 1.00 24.82 | 6 |
| MOTA | .1294 | | | A 164 | 30.247 | 27.655 | 60.198 | 1.00 24.51 | 6 |
| ATOM | 1295 | | | A 164 | 28.216 | 25.827 | 60.631 | 1.00 27.61 | 6 |
| ATOM | 1296 | CE2 | | A 164 | 28.065 | 26.808 | 59.662 | 1.00 25.67 | 5 |
| MOTA | 1297 | CZ | | A 164 | 29.078 | 27.718 | 59.451 | 1.00 25.63 | 6 |
| MOTA | 1298 | OH | | A 164 | 28.898 | 28.704 | 58.506 | 1.00 27.10 | 8 |
| ATOM | 1299 | С | | A 164 | 28.149 | 25.907 | 64.218 | 1.00 28.38 | 6 8 |
| ATOM | 1300 | 0 | | A 164 | 27.119 | 25.225 | 64.277 | 1.00 29.43 | 7 |
| ATOM | 1301 | N | | A 165 | 28.166 | 27.217 | 64.464 | 1.00 24.30 1.00 22.93 | 6 |
| MOTA | 1302 | CA | | A 165 | 26.941 | 27.969 | -64.754 | 1.00 22.93 | 6 |
| MOTA | 1303 | СВ | | A 165 | 26.985 | 28.649 | 66.143 | | 6 |
| MOTA | 1304 | CG2 | | A 165 | 25.765 | 29.559 | 66.312 | 1.00 16.15 1.00 20.78 | 6 |
| MOTA | 1305 | | | A 165 | 27.033 | 27.567 | 67.240 | | 6 |
| ATOM | 1306 | | | A. 165 | 27.185 | 28.101 | 68.650 63.657 | 1.00 15.49 | 6 |
| ATOM | 1307 | Ċ | | A 165 | 26.784 | 29.010 | 63.506 | 1.00 23.17 | 8 |
| MOTA | 1308 | 0 | | A 165 | 27.605 | 29.921 | | 1.00 24.20 | 7 |
| MOTA | 1309 | N | | A 166 | 25.709 | 28.871 | 62.895 61.749 | 1.00 24.20 | 6 |
| Mota | 1310 | CA | | A 166 | 25.478 | 29.726 | | 1.00 20.78 | 6 |
| MOTA | 1311 | CB | | A 166 | 25.314 | 28.809 | 60.548 59.256 | 1.00 17.84 | 6 |
| MOTA | 1312 | CG | | A 166 | 25.410 | 29.529 | | 1.00 19.93 | 8 |
| ATOM | 1313 | | | A 166 | 24.536 | 30.391 | 59.004 58.401 | 1.00 20.20 | 8 |
| MOTA | 1314 | | | A 166 | 26.366 | 29.231 | 58.491 | 1.00 17.84 | 6 |
| MOTA | 1315 | č | | A 166 | 24.290 | 30.570 | 61.895 | 1.00 22.79 | . 8 |
| ATOM | 1316 | 0 | | A 166 | 23.134 | 30.256 | 61.826 | 1.00 25.40 | 7 |
| MOTA | 1317 | N | LEU | A 167 | 24.583 | 31.952 | 62.085 62.250 | 1.00 25.76 | 6 |
| HOTE | 1318 | CA | | A 167 | 23.536 | 32.954 | 63.288 | 1.00 25.76 | 6 |
| MOTA | 1319 | CB | | A 167 | 23.963 | 33.991 | 64.674 | 1.00 26.65 | 6 |
| MOTA | 1320 | ÇĢ | LEU A | A 167 | 24.364 | 33.463 | 03.0/4 | 1.00 20.73 | • |

| ATOM | 1321 | CI | 1 LEU A 16 | 7 | 24.741 | 34.647 | 65.552 | 1.00 26.24 | _ |
|--------|------|-----|-------------|---|--------|------------------|------------------|------------|--------|
| MOTA | 1322 | | 2 LEU A 16 | | 23.225 | | 65.302 | | 6 |
| MOTA | 1323 | | LEU A 16 | | 23.162 | | | 1.00 23.45 | 6 |
| ATOM | 1324 | | LEU A 16 | | | | 60.951 | 1.00 26.37 | 6 |
| | 1325 | | | | 22.386 | | 60.971 | 1.00 25.95 | 8 |
| ATOM | | | ASP A 16 | | 23.726 | | 59.828 | 1.00 29.66 | 7. |
| ATOM- | 1326 | | | | 23.410 | 33.787 | 58.520 | 1.00 28.35 | 6 |
| MOTA | 1327 | _ | | | 24.057 | 32.987 | 57.390 | 1.00 33.29 | 6 |
| ATOM | 1328 | | | | 23.937 | 33.676 | 56.037 | 1.00 35.38 | 6 |
| MOTA | 1329 | | 1 ASP A .16 | | 24.892 | 34.388 | 55.659 | 1.00 39.48 | 8 |
| MOTA | 1330 | OD | 2-ASP A 16 | 8 | 22.893 | 33.531 | 55.364 | 1.00 33.40 | 8 |
| ATOM | 1331 | Ç | ASP A 16 | 8 | 21.906 | 33.614 | 58.408 | 1.00 28.74 | 6 |
| ATOM | 1332 | 0 | ASP A 16 | 8 | 21.354 | 32.648 | 58.948 | 1.00 26.21 | 8 |
| MOTA | 1333 | N | ALA A 16 | | 21.239 | 34.524 | 57.711- | | 7 |
| ATOM | 1334 | CA | ALA A 16 | 9 | 19.793 | 34.415 | 57.579 | 1.00 24.39 | |
| ATOM | 1335 | CB | | - | 19.233 | 35.640 | 56.879 | 1.00 22.75 | 6 |
| ATOM | 1336 | c | ALA A 16 | | 19.420 | 33.157 | | | 6 |
| ATOM | 1337 | õ | ALA A 16 | | 18.266 | | 56.813 | 1.00 24.37 | 6 - |
| ATOM | 1338 | N | HIS A 17 | | 20.405 | 32.752 | 56.824 | 1.00 22.34 | 8 |
| ATOM | 1339 | CA | | _ | | 32.542 | 56.156 | 1.00 25.78 | 7 |
| ATOM | 1340 | CB | HIS A 17 | | 20.180 | 31.327 | 55.375 | 1.00 25.20 | 6 |
| | 1341 | | | | 20.667 | 31.501 | 53.936 | 1.00 25.76 | 6 |
| MOTA | | CG | | | 20.122 | 32.711 | 53.245 | 1.00 29.08 | 6 |
| ATOM | 1342 | | 2 HIS A 17 | | 19.338 | 32.834 | 52.147 | 1.00 30.59 | 6 |
| ATOM | 1343 | | 1 HIS A 17 | | 20.384 | 33.995 | 53.675 | 1.00 30.77 | 7 |
| ATOM | 1344 | | 1 HIS A 17 | | 19.784 | 34.858 | 52.873 | 1.00 29.07 | 6 |
| ATOM | 1345 | | 2 HIS A 17 | | 19.143 | 34.180 | 51.939 | 1.00 32.19 | 7 |
| ATOM | 1346 | С | HIS A 17 | | 20.895 | 30.113 | 55.958 | 1.00 26.00 | 6 |
| ATOM | 1347 | 0 | HIS A 17 | | 21.913 | 30.234 | 56.637 | 1.00 25.76 | 8 |
| ATOM | 1348 | N | HIS A 17 | | 20.349 | 28.939 | 55.658 | 1.00 27.29 | 7 |
| MOTA | 1349 | CA | HIS A 17 | | 20.893 | 27.655 | 56.090 | 1.00 25.01 | 6 |
| MOTA | 1350 | CB | . HIS A 17 | 1 | 19.934 | 26.532 | 55.663 | 1.00 24.93 | 6 |
| MOTA | 1351 | CG | HIS A 17 | | 20.468 | 25.148 | 55.889 | 1.00 26.56 | 6 |
| MOTA | 1352 | | 2 HIS A 17 | | 20.674 | 24.123 | 55.028 | 1.00 22.34 | 6 |
| ATOM | 1353 | ND: | 1 HIS A 17 | 1 | 20.823 | 24.678 | 57.137 | 1.00 25.35 | 7 |
| MOTA | 1354 | CE: | l HIS A 17 | 1 | 21.222 | | . 57.036 | 1.00 22.68 | 6 |
| MOTA | 1355 | NE | 2 HIS A 17 | l | 21.140 | 23.062 | 55.767 | 1.00 24.13 | 7 |
| MOTA | 1356 | C | HIS A 17 | 1 | 22.267 | 27.413 | 55.471 | 1.00 24.74 | 6 |
| MOTA | 1357 | 0 | HIS A 17 | 1 | 22.540 | 27.863 | 54.356 | 1.00 28.22 | 8 |
| MOTA | 1358 | N | CYS A 17: | 2 | 23.131 | 26.705 | 56.190 | 1.00 23.03 | 7 |
| ATOM | 1359 | CA | CYS A 17 | 2 | 24.467 | 26.389 | 55.683 | 1.00 23.41 | 6 |
| ATOM | 1360 | CB | CYS A 17: | 2 | 25.497 | 26.474 | 56.812 | 1.00 19.31 | 6 |
| MOTA | 1361 | SG | CYS A 17: | | 25.005 | 25.631 | 58.318 | 1.00 16.78 | 16 |
| ATOM | 1362 | С | CYS A 17 | | 24.484 | 24.997 | 55.048 | 1.00 25.45 | 6 |
| MOTA | 1363 | 0 . | | | 25.203 | 24.098 | 55.483 | 1.00 24.47 | 8 |
| ATOM | 1364 | N | ASP A 17 | | 23.664 | 24.839 | 54.015 | 1.00 26.67 | 7 |
| ATOM | 1365 | CA | ASP A 17 | | 23.542 | 23.593 | 53.269 | 1.00 26.47 | 6 |
| ATOM | 1366 | CB | ASP A 17 | | 22.735 | 23.857 | 51.993 | 1.00 26.47 | |
| ATOM | 1367 | CG | ASP A 1 | | 23.281 | 25.030 | 51.179 | 1.00 25.33 | 6 6 |
| ATOM | 1368 | | ASP A 17. | | 22.539 | 25.558 | 50.330 | | |
| ATOM | 1369 | | ASP A 173 | | 24.454 | 25.417 | | 1.00 23.43 | 8 |
| ATOM | 1370 | c | ASP A 173 | | 24.872 | 22.932 | 51.372 52.922 | 1.00 29.38 | 8 |
| ATOM | 1371 | ō | ASP A 173 | | | | | 1.00 26.65 | 6 |
| ATOM | 1372 | N | GLY A 174 | | 24.940 | | | | 8 |
| | 1373 | CA | | | 25.926 | 23.737 | 52.793 | 1.00 25.24 | 7 |
| ATOM | | | GLY A 174 | | 27.227 | 23.198 | 52.447 | 1.00 23.11 | 6 |
| MOTA | 1374 | c | GLY A 174 | | 27.896 | 22.505 | 53.612 | 1.00 25.64 | 6 |
| ATOM | 1375 | 0 | GLY A 174 | | 28.443 | 21.408 | 53.462 | 1.00 27.67 | 8 |
| ATCM | 1376 | N | VAL A 175 | | 27.848 | 23.144 | 54.778 | 1.00 24.29 | 7 |
| MOTA | 1377 | CA | VAL A 175 | | 28.459 | 22.602 | 55.989 | 1.00 22.20 | 6 |
| MOTA | 1378 | CB | VAL A 175 | | 28.536 | 23.672 | 57.101 | 1.00 20.15 | 6 |
| MOTA | 1379 | | VAL A 175 | | 29.449 | 23.192 | 58.218 | 1.00 20.11 | 6 |
| MOTA | 1380 | | VAL A 175 | | 29.015 | 24.989 | 56.530 | 1.00 18.74 | 6 |
| ATOM | 1381 | С | VAL A 175 | | 27.647 | 21.409 | 56.505 | 1.00 22.85 | 6 |
| MOTA | 1382 | 0 | VAL A 175 | | 28.173 | 20.512 | 57.173: | 1.00 20.07 | 8 |
| MOTA | 1383 | N | GLN A 176 | | 26.356 | 21.404 | 56.203 | 1.00 24.12 | 7 |
| ATCM · | 1384 | CA | GLN A 176 | | 25.518 | 20.303 | 56.629 | 1.00 27.18 | 6 |
| MOTA | 1385 | CB | GLN A 176 | | 24.045 | 20.611 | 56.355 | 1.00 32.86 | 6 |
| ATOM | 1386 | CG | GLN A 176 | | 23084 | 19.483 | 56.726 | 1.00 36.04 | 6 |
| | | | | | | - · - · - | | | - |

| MOTA | 1387 | CD | GLN A | 176 | 21.620 | 19.862 | 56.537 | 1.00 38.36 | c |
|------|------|-----|---------|-----|--------|--------|---------|------------|---|
| ATOM | 1388 | | L GLN A | | 21.113 | 20.782 | 57.185 | 1.00 38.59 | 6 |
| ATOM | 1389 | | GLN A | | 20.934 | | | | 8 |
| | 1390 | C | GLN A | | | 19.151 | 55.649 | 1.00 38.81 | 7 |
| MOTA | | | | | 25.956 | 19.083 | 55.841 | 1.00 27.70 | 6 |
| MOTA | 1391 | 0 | GLN A | | 26.326 | 18.066 | 56.416 | 1.00 26.89 | 8 |
| MOTA | 1392 | N | GLU A | | 25.951 | 19.194 | 54.519 | 1.00 27.96 | 7 |
| ATOM | 1393 | CA | GLU A | | 26.343 | 18.062 | 53.698 | 1.00 31.16 | 6 |
| ATOM | 1394 | CB | GLU A | 177 | 26.395 | 18.460 | 52.220 | 1.00 30.37 | 6 |
| MOTA | 1395 | CG | GLU A | 177 | 26.353 | 17.256 | 51.287 | 1.00 36.20 | 6 |
| ATOM | 1396 | CD | GLU A | 177 | 26.273 | 17.626 | 49.818 | 1.00 40.70 | 6 |
| ATOM | 1397 | OE1 | GLU A | 177 | 27.322 | 17.967 | 49.234 | 1.00 46.78 | 8 |
| ATOM | 1398 | OE2 | GLU A | 177 | 25.155 | 17.590 | 49.250 | 1.00 39.39 | 8 |
| ATOM | 1399 | С | GLU A | | 27.702 | 17.516 | 54.137 | 1.00 31.66 | 6 |
| ATOM | 1400 | 0 | GLU A | | 27.868 | 16.317 | 54.356 | 1.00 32.81 | 8 |
| ATOM | 1401 | N | ALA A | | 28.663 | 18.419 | 54.287 | 1.00 32.81 | 7 |
| ATOM | 1402 | CA | ALA A | | 30.026 | 18.072 | 54.673 | | |
| ATOM | 1403 | СВ | ALA A | | 30.830 | 19.338 | | 1.00 31:63 | 6 |
| | 1404 | C | ALA A | | | | 54.856 | 1.00 30.96 | 6 |
| ATOM | | | | | 30.204 | 17.185 | 55.897 | 1.00 30.63 | 6 |
| ATOM | 1405 | 0 | ALA A | | 31.032 | 16.276 | 55.876 | 1.00 27.95 | 8 |
| ATOM | 1406 | N | PHE A | | 29.444 | 17.444 | 56.961 | 1.00 31.01 | 7 |
| ATOM | 1407 | CA | PHE A | | 29.590 | 16.656 | 58.184 | 1.00 31.34 | 6 |
| MOTA | 1408 | CB | PHE A | | 30.147 | 17.532 | 59.310 | 1.00 30.13 | 6 |
| ATOM | 1409 | ÇĞ | PHE A | | 31.189 | 18.505 | 58.858 | 1.00 27.78 | 6 |
| MOTA | 1410 | | PHE A | | 30.827 | 19.790 | 58.466 | 1.00 28.24 | 6 |
| ATOM | 1411 | | PHE A | | 32.522 | 18.124 | 58.766 | 1.00 28.33 | 6 |
| MOTA | 1412 | CE1 | PHE A | 179 | 31.778 | 20.688 | 57.988 | 1.00 26.68 | 6 |
| ATOM | 1413 | CE2 | PHE A | 179 | 33.487 | 19.013 | 58.285 | 1.00 28.79 | 6 |
| ATOM | 1414 | CZ | PHE A | 179 | 33.111 | 20.300 | 57.895 | 1.00 28.67 | 6 |
| ATOM | 1415 | С | PHE A | 179 | 28.300 | 16.003 | 58.664 | 1.00 32.06 | 6 |
| MOTA | 1416 | 0 | PHE A | 179 | 28.218 | 15.542 | 59.803 | 1.00 30.58 | 8 |
| ATOM | 1417 | N | TYR A | 180 | 27.305 | 15.960 | 57.787 | 1.00 34.25 | 7 |
| ATOM | 1418 | CA | TYR A | | 26.001 | 15.377 | 58.099 | 1.00 3B.60 | 6 |
| ATOM | 1419 | CB | TYR A | | 25.062 | 15.605 | 56.911 | 1.00 38.99 | 6 |
| ATOM | 1420 | CG | TYR A | | 23.593 | 15:453 | 57.220 | 1.00 37.91 | 6 |
| ATOM | 1421 | | TYR A | | 22.938 | 14.232 | 57.064 | 1.00 35.83 | 6 |
| ATOM | 1422 | | TYR A | | 21.589 | 14.103 | 57.373 | 1.00 39.20 | 6 |
| ATOM | 1423 | | TYR A | | 22.861 | 16.543 | 57.694 | 1.00 37.56 | 6 |
| ATOM | 1424 | CE2 | | | 21.518 | 16.430 | 58.007 | 1.00 40.28 | 6 |
| ATOM | 1425 | CZ | TYR A | | 20.882 | 15.211 | 57.848 | 1.00 41.92 | 6 |
| ATOM | 1426 | ОН | TYR A | | 19.549 | 15.110 | 58.188 | 1.00 41.92 | 8 |
| ATOM | 1427 | C | TYR A | | 26.133 | 13.110 | 58.382 | 1.00 40.28 | 6 |
| | 1428 | ō | TYR A | | 25.158 | | | | |
| ATOM | 1429 | N | ASP A | | | 13.192 | 58.680 | 1.00 39.27 | 8 |
| MOTA | 1430 | | | | 27.363 | 13.402 | 58.319 | 1.00 43.51 | 7 |
| ATOM | | CA | ASP A | | 27.638 | 11.994 | 58.519 | 1.00 45.89 | 6 |
| MOTA | 1431 | CB | ASP A | | 28.414 | 11.487 | 57.303 | 1.00 51.00 | 6 |
| ATOM | 1432 | CG | ASP A | | 28.830 | 10.050 | 57.436 | 1.00 56.84 | 6 |
| ATOM | 1433 | | ASP A | | 29.637 | 9.750 | 58.345 | 1.00 59.47 | 8 |
| ATOM | 1434 | | ASP A | | 28.348 | 9.221 | 56.629 | 1.00 60.73 | 8 |
| MOTA | 1435 | C | ASP A | | 28.398 | 11.665 | 59.804 | 1.00 44.75 | 6 |
| ATOM | 1436 | 0 | ASP A | | 28.257 | 10.568 | 60.350 | 1.00 44.69 | 8 |
| ATOM | 1437 | N | THR A | | 29.194 | 12.506 | 60.298 | 1.00 41.26 | 7 |
| ATOM | 1438 | CA | | | 29.975 | 12.337 | 61.495 | 1.00 39.51 | 6 |
| ATOM | 1439 | CB | THR A | 182 | 31.408 | 12.881 | 61.355 | 1.00 39.19 | 6 |
| MOTA | 1440 | OG1 | THR A | 182 | 32.171 | 12.508 | 62.505 | 1.00 37.82 | 8 |
| ATOM | 1441 | CG2 | THR A | 182 | 31395 | 14.397 | 61.232 | 1.00 40.12 | 6 |
| ATOM | 1442 | С | THR A | 182 | 29.370 | 12.910 | 62.759 | 1.00 38.58 | 6 |
| ATCM | 1443 | 0 | THR A | | 28.609 | 13.876 | 62.716 | 1.00 41.24 | 8 |
| ATOM | 1444 | N | ASP A | | 29.712 | 12.304 | 63.890 | 1.00 37.39 | 7 |
| ATOM | 1445 | CA | ASP A | | 29.211 | 12.773 | 65.171 | 1.00 39.24 | 6 |
| ATOM | 1446 | CB | ASP A | | 28.824 | 11.588 | 66.061 | 1.00 40.31 | 6 |
| ATOM | 1447 | CG | ASP A | | 30.010 | 10.723 | 66.433 | 1.00 41.64 | 6 |
| ATOM | 1448 | | ASP A | | 30.725 | 10.723 | 65.520 | 1.00 42.53 | 8 |
| ATOM | 1449 | | ASP A | | 30.221 | 10.494 | 67.640 | 1.00 42.46 | 8 |
| ATOM | 1450 | C | ASP A | | 30.286 | 13.621 | 65.853 | 1.00 40.34 | 6 |
| | 1451 | 0 | ASP A | | | 14.071 | 66.983 | 1.00 42.07 | 8 |
| ATOM | 1451 | N | GLN A | | 30.109 | 13.830 | 65.154 | 1.00 42.07 | 7 |
| ATCM | 1424 | 14 | GEMA W | 104 | 31.400 | 13.830 | -07.104 | 1.00 33.29 | , |

| ATO | M 1453 CA GLN A 184 | 32.506 | 14 625 | | | |
|------|---|-----------|----------------|--------|--------------|-----|
| ATO | M 1454 CB GLN A 184 | | 14.635 | 65.67 | 1 1.00 37.08 | 3 6 |
| ATO | | 33.830 | 14.252 | 64.994 | 4 1.00 33.77 | è |
| ATO | CDW Y 10d | 34.229 | 12.804 | 65.166 | 1.00 33.63 | |
| ATO | | 35.599 | 12.499 | 64.593 | 1.00 32.74 | • |
| | APT CEN V TON | 35.853 | 12.704 | 63.413 | | |
| ATO | TO CENT I TOG | 36.490 | 11.999 | 65.436 | | 8 |
| ATO | - CTM N 704 | 32.222 | 16.110 | | | 7 |
| ATO | M 1460 O GLN A 184 | 32.803 | | 65.403 | | 6 |
| ATO | M 1461 N VAL A 185 | 31.329 | 16.994 | 66.034 | | 8 |
| ATO | M 1462 CA VAL A 185 | | 16.372 | 64.456 | 1.00 33.14 | 7 |
| ATO | | 30.984 | 17.740 | 64.119 | 1.00 32.40 | 6 |
| ATO | | 31.308 | 18.052 | 62.641 | 1.00 33.03 | 6 |
| ATO | cor AMD Y 100 | 31.009 | 19.520 | 62.331 | | |
| ATON | *********************************** | 32.773 | 17.738 | 62.357 | 1.00 34.58 | |
| | | 29.508 | 17.972 | 64.360 | | 6 |
| ATON | v vial is 100 | 28.680 | 17.124 | 64.038 | | 6 |
| ATOM | 11.2 11 100 | | 19.119 | | | 8 |
| ATOM | | | 19.463 | 64.946 | | 7 |
| ATOM | 1 1470 CB PHE A 186 | | | 65.207 | | ·6 |
| ATOM | 1471 CG PHE A 186 | | 19.532 | 66.716 | | 6 |
| ATOM | 1472 CD1 PHE A 186 | | 19.617 | 67.066 | 1.00 31.59 | 6 |
| ATOM | | | 18.901 | 68.153 | 1.00 30.54 | 6 |
| ATOM | | 25.179 | 20.395 | 66.308 | 1.00 31.50 | 6 |
| MOTA | | | 18.951 | 68.478 | 1.00 33.28 | |
| | 21 100 | 23.815 | 20.457 | 66.622 | 1.00 33.04 | 6 |
| ATOM | | | 15.733 | 67.708 | 1.00 33.04 | 6 |
| ATOM | | | 20.798 | 64.551 | 1.00 32.35 | 6 |
| ATOM | 2.12 N 100 | | 21.789 | 64.751 | 1.00 30.37 | 6 |
| MOTA | | | 20.809 | | 1.00 31.32 | 8 |
| MOTA | 1480 CA VAL A 187 | | 22.015 | 63.752 | 1.00 31.14 | 7 |
| MOTA | 1481 CB VAL A 187 | | | 63.063 | 1.00 32.05 | 6 |
| ATOM | 1482 CG1 VAL A 187 | | 21.805 | 61.525 | 1.00 33.54 | 6 |
| ATOM | 1483 CG2 VAL A 187 | | 23.081 | 60.813 | 1.00 32.07 | ε |
| MOTA | 1484 C VAL A 187 | | 1.389 | 61.056 | 1.00 35.44 | 6 |
| ATOM | 1485 O VAL A 187 | 24.638 2 | 2.439 | 63.524 | 1.00 31.47 | 6 |
| ATOM | 1486 N LEU A 188 | | 1.686. | 63.410 | 1.00 29.06 | 8 |
| ATOM | | 24.579 2 | 3.638 | 64.090 | 1.00 29.44 | 7 |
| ATOM | | | 4.228 | 64.551 | 1.00 29.39 | 6 |
| | | 23.433 2 | 4.665 | 66.009 | 1.00 29.52 | |
| ATOM | 1489 CG LEU A 188 | 22.293 2 | | 66.458 | 1.00 27.92 | 6 |
| ATOM | 1490 CD1 LEU A 188 | | | 66.414 | 1.00 27.92 | 6 |
| MOTA | 1491 CD2 LEU A 188 | | | 67.861 | 1.00 25.87 | 6 |
| ATOM | 1492 C LEU A 188 | | | 63.675 | 1.00 27.69 | 6 |
| ATOM | 1493 O LEU A 188 | | | | 1.00 31.89 | 6 |
| ATOM | 1494 N SERA 189 | | - | 63.388 | 1.00 31.50 | 8 |
| ATOM | 1495 CA SER A 189 | | | 63.250 | 1.00 29.93 | 7 |
| MOTA | 1496 CB SER A 189 | | | 52.390 | 1.00 24.65 | 6 |
| ATOM | 1497 OG SER A 189 | | 6.411 | 50.942 | 1.00 22.40 | 6 |
| ATOM | 1498 C SER A 189 | | | 50.083 | 1.00 19.12 | 8 |
| MOTA | 1499 O SER A 189 | | | 52.540 | 1.00 27.00 | 6 |
| MOTA | 1500 N LEU A 190 | | | 52.577 | 1.00 26.72 | 8 |
| ATOM | 1501 CA LEU A 190 | | 3.783 <i>6</i> | 2.669 | 1.00 27.41 | 7 |
| ATOM | 1502 CB LEU A 190 | | | 2.735 | 1.00 29.68 | 6 |
| MOTA | ======================================= | 19.185 30 | 0.682 6 | 3.771 | 1.00 29.84 | 6 |
| | | 19.108 30 | | 5.264 | 1.00 26.79 | 6 |
| ATOM | 1504 CD1 LEU A 190 | | | 6.045 | 1.00 23.44 | |
| ATOM | 1505 CD2 LEU A 190 | 17.881 29 | | 5.546 | 1 00 22 62 | 6 |
| ATOM | 1506 C LEU A 190 | 19.046 30 | | | 1.00 27.63 | 6 |
| ATOM | 1507 O LEU A 190 | | | | 1.00 29.58 | 6 |
| ATOM | 1508 N HIS A 191 | 17.864 30 | | | 1.00 32.40 | 8 |
| ATOM | 1509 CA HIS A 191 | | | 0.727 | 1.00 29.61 | 7 |
| MOTA | 1510 CB HIS A 191 | | | 9:368 | 1.00 29.72 | 6 |
| ATOM | 1511 CG HIS A 191 | 10 000 | 839 5 | 8.432 | 1.00 26.47 | 6 |
| ATOM | 1512 CD2 HIS A 191 | | .392 5 | 8.504 | 1.00 28.18 | 6 |
| ATOM | 1513 ND1 HIS A 191 | 18.918 27 | | 8.940 | 1.00 28.88 | 6 |
| ATOM | | | .921 5 | B.118 | 1.00 31.00 | 7 |
| ATOM | | 16.938 26 | .614 5 | 8.312 | 1.00 30.54 | 6 |
| ATOM | | 18.095 26 | | 3.810 | 1.00 27.21 | 7 |
| | 1516 C HIS A 191 | 16.329 30 | | | 1.00 28.05 | 6 |
| ATOM | 1517 O HIS A 191 | | | .535 | 1.00 27.81 | 8 |
| MOTA | 1518 N GLN A 192 | | | | 1.00 29.39 | 7 |
| • | • • • • • | | • | | 63.39 | • |

91/263 Figure 17-24

| MOTA | 1519 | C2 | GLN A 192 | | 14.886 | 31.494 | 57.008 | 1.00 28.21 | 6 |
|--------------|--------------|----------|------------------------------|---|------------------|------------------|------------------|--------------------------|---------|
| ATOM | 1520 | | | | 15.016 | 32.416 | 55. 796 | | 6 |
| ATOM | 1521 | | | | 15.622 | | 56.124 | 1.00 21.66 | 6 |
| MOTA | 1522 1523 | | | | 15.701 | | 54.921 | 1.00 22.22 | 6 |
| MOTA MOTA | 1524 | | Cl GLN A 192 C2 GLN A 192 | | 14.684 | | 54.428 54.434 | 1.00 23.38 | 8 |
| MOTA | 1525 | | GLN A 192 | | 16.914 14.435 | | 56.570 | 1.00 22.97 1.00 32.71 | 7 |
| MOTA | 1526 | | GLN A 192 | ٠ | 15.157 | 29.403 | 55.853 | 1.00 32.71 | 6 8 |
| ATOM | 1527 | | SER A 193 | | 13.249 | 29.694 | 57.011 | 1.00 34.44 | 7 |
| MOTA | 1528 | | | | 12.751 | 28.376 | 56.650 | 1.00 33.28 | 6 |
| ATOM | 1529 | | | - | 11.264 | 28.249 | 56.961 | 1.00 33.25 | 6 |
| MOTA | 1530 | | | | 10.786 | 26.987 | 56.540 | 1.00 31.52 | 8 |
| MOTA MOTA | 1531 1532 | | SER A 193 SER A 193 | | 12.974 | 28.150 | 55.171 | 1.00 34.79 | 6 |
| ATOM | 1532 | | PRO A 194 | | 12.775 13.404 | 29.051 26.938 | 54.356 54.803 | 1.00 33.74 1.00 37.57 | 8 |
| ATOM | 1534 | | | | 13.689 | 25.775 | 55.658 | 1.00 37.37 | 7 6 |
| MOTA | 1535 | | | | 13.654 | 26.600 | 53.403 | 1.00 37.81 | 6 |
| MOTA | 1536 | CB | PRO A 194 | | 14.248 | 25.194 | 53.498 | 1.00 39.30 | 6 |
| MOTA | 1537 | CG | PRO A 194 | | 14.840 | 25.163 | 54.916 | 1.00 39.09 | 6 |
| ATOM | 1538 | C | PRO A 194 | | 12.340 | 26.617 | 52.638 | 1.00 36.81 | 6 |
| ATOM | 1539 1540 | O N | PRO A 194 GLU A 195 | | 12.317 | 26.443 | 51.425 | 1.00 34.09 | 8 |
| ATOM ATOM | 1541 | CA | GLU A 195 | | 11.246 9.928 | 26.835 26.866 | 53.364 52.750 | 1.00 39.25 1.00 41.54 | 7 |
| ATOM | 1542 | CB | GLU A 195 | | 8.843 | 26.600 | 53.812 | 1.00 41.34 | 6 6 |
| ATOM | 1543 | CG | GLU A 195 | | 8.360 | 27.811 | 54.608 | 1.00 53.30 | 6 |
| ATOM | 1544 | CD | GLU A 195 | | 7.160 | 28.502 | 53.960 | 1.00 55.91 | 6 |
| ATOM | 1545 | OE: | | | 6.735 | 29.571 | | 1.00 55.14 | 8 |
| ATOM | 1546 1547 | OE2 | GLU A 195 GLU A 195 | | 6.631 | 27.966 | 52.956 | 1.00 57.75 | 8 |
| ATOM ATOM | 1548 | 0 | GLU A 195 | | 9.700 8.651 | 28.208 28.431 | 52.047 51.452 | 1.00 39.50 1.00 40.21 | 6 |
| ATOM | 1549 | N | TYR A 196 | | 10.689 | 29.096 | 52.098 | 1.00 40.21 | 8 7. |
| ATOM | 1550 | CA | TYR A 196 | | 10.549 | 30.379 | 51.434 | 1.00 35.50 | 6 |
| ATOM | 1551 | CB | TYR A 196 | | 9.602 | 31.274 | 52.245 | 1.00 36.36 | 6 |
| MOTA | | . CG | TYR A 196 | | 10.175 | 31.816 | 53.538 | 1.00 37.28 | 6 |
| ATOM | 1553 | | TYR A 196 | | 11.120 | 32.848 | 53.527 | 1.00 35.42 | 6 |
| ATOM ATOM | 1554 1555 | CE1 | - · · · · · | | 11.637 9.764 | 33.366 31.311 | 54.706 54.776 | 1.00 33.10 1.00 36.75 | 6 6 |
| ATOM | 1556 | CE2 | | | 10.279 | 31.825 | 55.968 | 1.00 35.26 | 6 |
| ATOM | 1557 | CZ | TYR A 196 | | 11.213 | 32.856 | 55.922 | 1.00 35.84 | 6 |
| MOTA | 1558 | OH | TYR A 196 | | 11.704 | 33.401 | 5 7.087 . | 1.00 37.09 | 8 |
| MOTA | 1559 | С | TYR A 196 | | 11.878 | 31.097 | 51.188 | 1.00 34.89 | 6 |
| MOTA | 1560 | 0 | TYR A 196 | | 11.896 | 32.256 | 50.764 | 1.00 31.61 | 8 |
| ATOM ATOM | 1561 1562 | N CA | ALA A 197 ALA A 197 | | 12.991 14.297 | 30.416 31.041 | 51.437 51.242 | 1.00 34.39 1.00 34.82 | 7 6 |
| ATOM | 1563 | CB. | ALA A 197 | | 14.684 | 31.826 | 52.489 | 1.00 34.82 | 6 |
| ATOM | 1564 | C | ALA A 197 | | 15.418 | 30.075 | 50.887 | 1.00 36.59 | 6 |
| ATOM | 1565 | 0 | ALA A 197 | | 15.407 | 28.903 | 51.291 | 1.00 37.46 | 8 |
| ATOM | 1566 | N | PHE A 198 | | 16.388 | 30.584 | 50.133 | 1.00 36.22 | 7 |
| ATOM | 1567 | CA | PHE A 198 | | 17.548 | 29.802 | 49.722 | 1.00 37.68 | 6 |
| ATOM ATOM | 1568 1569 | CB CG | PHE A 198 PHE A 198 | | 18.597 19.810 | 30.729 30.013 | 49.109 48.578 | 1.00 40.89 1.00 43.59 | 6 6 |
| ATOM | 1570 | | PHE A 198 | | 19.783 | 29.404 | 47.325 | 1.00 44.74 | 6 |
| ATOM | 1571 | | PHE A 198 | | 20.970 | 29.929 | 49.336 | 1.00 41.86 | 6 |
| ATOM | 1572 | | PHE A 198 | | 20.894 | 28.729 | 46.833 | 1.00 41.42 | 6 |
| MOTA | 1573 | | PHE A 198 | | 22.079 | 29. 251 | 48.849 | 1.00 43.30 | 6 |
| MOTA | 1574 | cz | PHE A 198 | | 22.040 | 28.652 | 47.595 | 1.00 41.86 | 6 |
| MOTA | 1575 1576 | C | PHE A 198 | | 18.139 | 29.140 | 50.967 | 1.00 37.00 | 6 |
| ATOM | 1576 1577 | O N | PHE A 198 PRO A 199 | | 18.166 18.641 | 29.754 | 52.036 50.848 | 1.00 36.43 1.00 37.63 | 8 7 |
| ATOM ATOM | 1578 | CD | PRO A 199 | | 19.298 | 27.892 27.238 | 51.997 | 1.00 37.63 | 6 |
| ATOM | 1579 | CA | PRO A 199 | | 18.727 | 27.008 | 49.673 | 1.00 36.52 | 6 |
| ATOM | 1580 | CB | PRO A 199 | | 19.702 | 25.936 | 50.138 | 1.00 34.96 | 6 |
| ATOM | 1581 | CG | PRO A 199 | | 19.281 | 25.770 | 51.565 | 1.00 34.57 | 6 |
| ATOM · | 1582 | C | PRO A 199 | | 17.409 | 26.380 | 49.222 | 1.00 35.72 | 6 |
| ATOM | 1583 | O N | PRO A 199 | | 17.386 | 25.663 | 48.225 | 1.00 37.36 | 8 |
| MOTA | 1584 | N | PHE A 200 | | 16.331 | 26.638 | 49.962 | 1.00 33.78 | 7 |

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| ATC | OM 1585 CA PHE A 200 | 15 004 04 000 |
|------------|---|--|
| PTA | OM 1586 CB PHE A 200 | 15.004 26.090 49.662 1.00 32.15 6 |
| ATO | | 14.562 26.381 48.222 1.00 28.39 6 |
| ATO | OM 1588 CD1 PHE A 200 | 14.600 27.827 47.835 1.00 26.29 6 15.749 28.385 47.396 1.00 24.29 |
| ATC | OM 1589 CD2 PHE A 200 | 12 466 - 1200 1.00 24.82 6 |
| ATC | OM- 1590 CE1 PHE A 200 | 20.023 47.966 1.00 28.04 6 |
| PPA | OM 1591 CE2 PHE A 200 | 13.767 29.712 46.882 1.00 25.68 6 |
| ATC | M 1592 CZ PHE A 200 | 13.475 29.955 47.557 1.00 27.03 6 |
| ATC | | 14.626 30.498 47.013 1.00 24.90 6 |
| ĀTC | | 14.947 24.574 49.842 1.00 32.66 6 |
| ATC | | 13.925 24.033 50.264 1.00 31.22 8 |
| ATO | CD0 11 EQ1 | 16.043 23.896 49.499 1.00 33.60 7 |
| ATO | 020 11 201 | 10.128 22.438 49.585 1.00 30.86 6 |
| ATO | 42 020 A 201 | 17.213 21.931 48.637- 1.00 32.98 6 |
| ATO | 00 000 1, 201 | 16.879 22.182 47.175 1.00 33.52 6 |
| ATO | | 18.012 21.864 46.232 1 00 34 55 |
| ATO | | 18.396 20.678 46.117 1.00 36.35 |
| ATO | | 18.523 22.814 45.605 1.00 36 52 6 |
| ATO | | 10.369 21.911 50.981 1.00 28.52 6 |
| ATO | 020 11 201 | 15.537 21.199 51.520 1.00 28 91 |
| ATO | 210 11 202 | 17.511 22.239 51.566 1 00 31 64 |
| ATO | | 1/./95 21.780 52.917 1.00 32 34 6 |
| ATO | 1 | 19.276 21.432 53.092 1.00 36.91 6 |
| ATOM | 55 DID A 202 | 19.789 20.226 52.307 1.00 43 74 6 |
| ATON | | 20.212 20.590 50.891 1 00 49 31 |
| ATON | | 20.952 19.428 50.227 1.00 49 34 |
| ATOM | 202 | 21.504 19.802 48.895 1.00 49 89 |
| ATOM | | 17.421 22.849 53.937 1.00 30.55 6 |
| ATOM | | 16.877 23.890 53.586 1.00 26.55 8 |
| ATOM | | 17.710 22.571 55.203 1.00 30 59 7 |
| ATOM | 11 205 | 17.422 23.519 56.259 1.00 30 24 6 |
| ATOM | - 021 11 203 | 16.216 23.210 57.125 1.00 29 23 |
| ATOM | 1540 | 13.915 23.975 58.041 1.00 32 90 6 |
| ATOM | 1. 1. 209 | 15.526 22.104 56.866 1 00 26 32 7 |
| ATOM | 1.1.0 1. 204 | 14.344 21.779 57.657 1.00 23 25 6 |
| ATOM | | . 13.366 20.917 56.863 1.00 21.25 6 |
| ATOM | 1620 CG PHE A 204 1621 CD1 PHE A 204 | 12.855 21.573 55.635 1 00 18 60 6 |
| ATOM | 1622 CD2 PHE A 204 | 13.605 21.560 54.461 1.00 16.43 6 |
| ATOM | 1623 CE1 PHE A 204 | 11.654 22.273 55.664 1.00 14.82 6 |
| ATOM | 1624 CE2 PHE A 204 | 13.168 22.245 53.333 1.00 16.91 6 |
| ATOM | 1625 CZ PHE A 204 | 11.206 22.962 54.544 1.00 15.28 6 |
| ATOM | 1626 C PHE A 204 | 11.965 22.952 53.375 1.00 18.34 6 |
| ATOM | 1627 O PHE A 204 | 14.626 21.094 58.979 1.00 23.72 6 |
| ATOM | 1628 N LEU A 205 | 13.5/8 20.318 59.118 1.00 22.68 8 |
| ATOM | 1629 CA LEU A 205 | 13.760 21.376 59.942 1.00 20.94 7 |
| ATOM | 1630 CB LEU A 205 | 13.87/ 20.818 61.272 1.00 24.83 6 |
| ATOM | 1631 CG LEU A 205 | 12.678 21.259 52.110 1.00 21.29 6 |
| ATOM | 1632 CD1 LEU A 205 | 12.672 20.811 53.568 1.00 22.67 6 |
| ATOM | 1633 CD2 LEU A 205 | 14.011 21.182 34.245 1.00 19.76 6 11.478 21.456 64.275 1.00 20.52 |
| ATOM | 1634 C LEU A 205 | 14 000 |
| ATOM | 1635 O LEU A 205 | 14.002 19.293 61.303 1.00 28.79 6 14.443 18.730 62.310 1.00 28.59 6 |
| ATOM | 1636 N GLU A 206 | 13 605 |
| ATOM | 1637 CA GLU A 206 | 13.625 18.628 60.211 1.00 33.52 7 13.693 17.166 60.142 1.00 39.79 |
| ATOM | 1638 CB GLU A 206 | 10 776 |
| ATOM | 1639 CG GLU A 206 | 11 22 |
| ATOM | 1640 CD GLU A 206 | 17 01. 17.000 33.204 1.00.30.73 6 |
| ATOM | 1641 OE1 GLU A 206. | 2 |
| ATOM | 1642 OE2 GLU A 206 | 11 930 10 700 57 550 |
| ATOM | 1643 C GLU A 206 | 15 114 16 674 50 |
| ATOM | 1644 O GLU A 206 | 15 403 15 544 60 |
| ATOM | 1645 N GLU A 207 | 15 002 |
| MOTA | 1646 CA GLU A 207 | 17 305 18 300 |
| MOTA | 1647 CB GLU A 207 | 17 776 10 740 57 77 77 90 6 |
| ATOM . | 1648 CG GLU A 207 | 16 992 10 155 55 |
| ATOM | 1649 CD GLU A 207 | 16 979 10 453 55 773 100 33 |
| ATOM | 1650 OE1 GLU A 207 | |
| | dao a 207 | 18.071 20.016 55.537 1.00 35.44 8 |

| MOTA | 1651 | OE2 | GLU A 207 | 15.870 | 19.891 | 55.389 | 1.00 34.62 | 8 |
|-------|------|-------------|-----------|--------|--------|----------------|------------|---|
| | | | | | | 60.134 | 1.00 36.18 | 6 |
| MOTA | 1652 | C | GLU A 207 | 18.139 | 17.239 | | | |
| ATOM | 1653 | 0 | GLU A 207 | 18.560 | 18.303 | 60.590 | 1.00 34.81 | 8 |
| | 1654 | N | ILE A 208 | 18.381 | 16.059 | 60.701 | 1.00 34.45 | 7 |
| ATOM | | | | | | | | |
| ATOM | 1655 | CA | ILE A 208 | 19.164 | 15.965 | 61.932 | 1.00 38.53 | 6 |
| | 1656 | CB | ILE A 208 | 18.260 | 15.511 | 63.117 | 1.00 41.12 | 6 |
| ATOM | | | | | | | | |
| MOTA | 1657 | CG2 | ILE A 208 | 19.097 | 15.273 | 64.375 | 1.00 41.36 | 6 |
| ATOM | 1658 | CG1 | ILE A 208 | 17.193 | 16,581 | 63.383 | 1.00 42.21 | 6 |
| | | | | | | 64.560 | 1.00 44.81 | 6 |
| ATOM | 1659 | CD1 | | 16.291 | 16.286 | | | |
| MOTA | 1660 | C | ILE A 208 | 20.407 | 15.074 | 61.876 | 1.00 36.66 | 6 |
| | 1661 | 0 | ILE A 208 | 21.243 | 15.110 | 62.775 | 1.00 34.03 | 8 |
| ATOM | | | | | | | | |
| ATOM | 1662 | N | GLY A 209 | 20.540 | 14.284 | 60.822 | 1.00 36.80 | 7 |
| ATOM | 1663 | CA | GLY A 209 | 21.703 | 13.428 | 60.728 | 1.00 38.99 | 6 |
| | | • | | 21.509 | 12.246 | 59.805 | 1.00 40.93 | 6 |
| ATOM. | 1664 | С | GLY A 209 | | | | | |
| ATOM | 1665 | 0 | GLY A 209 | 20.477 | 12.124 | 59.145 | 1.00 40.26 | 8 |
| ATOM | 1666 | N | GLU A 210 | 22.508 | 11.370 | 59.775 | 1.00 42.16 | 7 |
| | | | | | | | - | |
| MOTA | 1667 | CA | GLU A 210 | 22.492 | 10.185 | 58.930 | 1.00 43.30 | 6 |
| ATOM | 1668 | CB | GLU A 210 | 22.810 | 10.586 | 57.488 | 1.00 47.08 | 6 |
| | | CG | GLU A 210 | 22.826 | 9.453 | 56.478 | 1.00 53.90 | 6 |
| ATOM | 1669 | | | | | | | |
| MOTA | 1670 | CD | GLU A 210 | 23.256 | 9.915 | 55.089 | 1.00 56.27 | 6 |
| ATOM | 1671 | OE1 | GLU A 210 | 24.412 | 10.371 | 54.941 | 1.00 56.19 | 8 |
| | | OE2 | | 22.437 | 9.826 | 54.145 | 1.00 60.28 | 8 |
| MOTA | 1672 | | | | | | | |
| MOTA | 1673 | С | GLU A 210 | 23.583 | 9.276 | 59.473 | 1.00 41.47 | 6 |
| ATOM | 1674 | 0 | GLU A 210 | 24.750 | 9.457 | 59.152 | 1.00 43.97 | 8 |
| | | | | 23.203 | 8.307 | 60.299 | 1.00 39.97 | 7 |
| ATOM | 1675 | N | GLY A 211 | | | | | |
| ATOM | 1676 | CA | GLY A 211 | 24.181 | 7.405 | 60.885 | 1.00 37.34 | 6 |
| MOTA | 1677 | С | GLY A 211 | 24.642 | 7.952 | 62.224 | 1.00 37.84 | 6 |
| | | | | 23.820 | 8.408 | 63.019 | 1.00 37.30 | 8 |
| MOTA | 1678 | 0 | GLY A 211 | | | | | |
| ATOM | 1679 | N | LYS A 212 | 25.948 | 7.910 | 62.485 | 1.00 38.52 | 7 |
| ATOM | 1680 | CA | LYS A 212 | 26.490 | 8.440 | 63.733 | 1.00 38.29 | 6 |
| | | | LYS A 212 | 28.020 | 8.359 | 63.731 | 1.00 40.54 | 6 |
| ATOM | 1681 | CB | | | | | | |
| MOTA | 1682 | CG | LYS A 212 | 28.570 | 6.950 | 63.675 | 1.00 46.39 | 6 |
| MOTA | 1683 | CD | LYS A 212 | 28.149 | 6.147 | 64.910 | 1.00 51.59 | 6 |
| | | | LYS A 212 | 28.556 | 4.676 | 64.809 | 1.00 52.77 | 6 |
| MOTA | 1684 | CE | | | | | | |
| ATOM | 1685 | NZ | LYS A 212 | 30.030 | 4.478 | 64.662 | 1.00 55.48 | 7 |
| MOTA | 1686 | С | LYS A 212 | 26.061 | 9.897 | 63.866 | 1.00 37.68 | 6 |
| | | | LYS A 212 | 25.814 | 10.389 | 64.962 | 1.00 34.75 | 8 |
| ATOM | 1687 | 0 | | | | | | |
| ATOM | 1688 | N | GLY A 213 | 25.956 | 10.574 | 62.728 | 1.00 38.89 | 7 |
| ATOM | 1689 | CA | GLY A 213 | 25.577 | 11.975 | 62.724 | 1.00 43.58 | 6 |
| | | | GLY A 213 | 24.126 | 12.295 | 63.020 | 1.00 43.99 | 6 |
| ATOM | 1690 | С | | | | | | |
| ATOM | 1691 | 0 | GLY A 213 | 23.737 | 13.464 | 63.024 | 1.00 44.67 | 8 |
| ATOM | 1692 | N | LYS A 214 | 23.321 | 11.268 | 63.265 | 1.00 46.02 | 7 |
| | 1693 | | LYS A 214 | 21.907 | 11.467 | 63.562 | 1.00 45.61 | 6 |
| MOTA | | CA | | | | | | |
| MOTA | 1694 | $^{\rm CB}$ | LYS A 214 | 21.168 | 10.130 | 63.469 | 1.00 47.77 | 6 |
| MOTA | 1695 | CG | LYS A 214 | 19.675 | 10.252 | 63.249 | 1.00 49.25 | 6 |
| | 1696 | CD | LYS A 214 | 19.078 | 8.901 | 62.911 | 1.00 51.64 | 6 |
| MOTA | | | | | | | 1.00 54.30 | 6 |
| MOTA | 1697 | CE | LYS A 214 | 17.637 | 9.038 | 62.440 | | |
| MOTA | 1698 | NZ | LYS A 214 | 17.030 | 7.727 | 62.034 | 1.00 56.09 | 7 |
| | 1699 | С | LYS A 214 | 21.809 | 12.047 | 64.970 | 1.00 44.22 | 6 |
| ATOM | | | | | | | 1.00 45.04 | 8 |
| ATOM | 1700 | 0 | LYS A 214 | 22.210 | 11.410 | 65.942 | | |
| MOTA | 1701 | N | GLY A 215 | 21.292 | 13.266 | 65.074 | 1.00 42.89 | 7 |
| | 1702 | CA | GLY A 215 | 21.193 | 13.904 | 66.373 | 1.00 40.20 | 6 |
| MOTA | 1702 | | | 21.133 | | | 1.00 39.90 | 6 |
| ATOM | 1703 | С | GLY A 215 | 22.295 | 14.931 | 66.600 | | |
| MOTA | 1704 | 0 | GLY A 215 | 22.356 | 15.548 | 67.668 | 1.00 40.12 | 8 |
| | 1705 | N | TYR A 216 | 23.175 | 15.111 | 65.612 | 1.00 38.49 | 7 |
| MOTA | | | | | | | 1.00 35.91 | 6 |
| MOTA | 1706 | CA | TYR A 216 | 24.261 | 16.086 | 65.726 | | |
| MOTA | 1707 | CB | TYR A 216 | 25.632 | 15.421 | 65.618 | 1.00 36.47 | 6 |
| | - | CG | TYR A 216 | 25.935 | 14.461 | 66.738 | 1.00 39.54 | 6 |
| MOTA | 1708 | | | | | | | 6 |
| MOTA | 1709 | CD1 | TYR A 216 | 25.296 | 13.220 | 66.810 | 1.00 40.62 | |
| ATOM | 1710 | CE1 | TYR A 216 | 25.561 | 12.333 | 67.849 | 1.00 41.58 | 6 |
| | | CD2 | TYR A 216 | 26.852 | 14.795 | 67.739 | 1.00 39.20 | 6 |
| MOTA | 1711 | | | | | | | 6 |
| MOTA | 1712 | CE2 | TYR A 216 | 27.124 | 13.915 | 68.78 6 | 1.00 40.87 | |
| ATOM | 1713 | CZ | TYR A 216 | 26.475 | 12.685 | 68.833 | 1.00 41.86 | 6 |
| | | OH | TYR A 216 | 26.743 | 11.802 | 69.852 | 1.00 43.04 | 8 |
| ATOM | 1714 | | | | | | 1.00 34.21 | 6 |
| MOTA | 1715 | С | TYR A 216 | 24.182 | 17.215 | 64.709 | | |
| ATOM | 1716 | 0 | TYR A 216 | 25.194 | 17.832 | 64.375 | 1.00 33.37 | 8 |
| VII | | - | | | | • | | |

| ATO: | M 1717 N ASNA 217 | 22.97 | 6 17 47 | | | |
|--------|----------------------|---------|----------|----------|------------|-----|
| ATO | M 1718 CA ASN A 217 | | | | 1.00 33.8 | 3 |
| ATO | | 22.72 | | 8 63.267 | 1.00 30.20 | 3 |
| | A Z1/ | 22.69 | 9 18.05 | 7 61.823 | 3.00 00.20 | • |
| ATO | M 1720 CG ASN A 217 | 22.45 | | | | 1 |
| ATO | M 1721 OD1 ASN A 217 | | | | 1.00 25.6 | ì. |
| ATO | M 1722 ND2 ASN A 217 | 21.35 | | 60.719 | 1.00 25.00 | 5 |
| | 11DIV A 217 | 23.50 | 1 19.558 | | 2.00 25.00 | , |
| ATO | M 1723 C ASN A 217 | 21.36 | | | | 3 |
| ATON | M 1724 O ASN A 217 | | | | 1.00 29.09 | • |
| | A 21/ | 20.43 | 3 18.351 | 63.885 | 1.00 26.93 | |
| MOTA | 220 11 210 | 21.263 | 3 20.440 | | | • |
| ATOM | M 1726 CA LEU A 218 | | | | |) |
| ATOM | | 20.010 | | 64.089 | 1.00 25.33 | ı |
| | 220 R 218 | 20.026 | 5 21.379 | 65.590 | | , |
| ATOM | 1 1728 CG LEU A 218 | 18.729 | | | | |
| · ATOM | 1 1729 CD1 LEU A 218 | | | | 1.00 21.00 | 1 |
| | | 19.100 | | 67.695 | 1.00 18.62 | |
| ATOM | 11 210 | 17.872 | 22.675 | | 1.00 18.02 | , |
| ATOM | 1731 C LEU A 218 | | | | 1.00 18.48 | |
| ATOM | 1732 O LEU A 218 | 19.785 | | 63.325 | 1.00 25.04 | |
| | | 20.596 | 23.287 | 63.415 | 1.00 25.23 | |
| ATOM | | 18.681 | | | 1.00 25.23 | |
| ATOM | 1734 CA ASN A 219 | | | | 1.00 28.44 | • |
| ATOM | | 18.310 | | 61.829 | 1.00 28.76 | |
| | | 17.809 | 23.298 | 60.417 | 1 00 05 10 | , |
| ATOM | 1736 CG ASN A 219 | 18.748 | | | 1.00 25.69 | • |
| MOTA | 1737 OD1 ASN A 219 | | | 59.646 | 1.00 26.10 | 6 |
| ATOM | 1738 ND2 ASN A 219 | 19.927 | 22.708 | 59.505 | 1.00 28.53 | |
| | | 18.220 | 21.311 | 59.114 | 3.00 28.33 | 8 |
| MOTA | 1739 C ASN A 219 | 17.129 | | 33.114 | 1.00 26.97 | 7 |
| ATOM | 1740 O ASN A 219 | | 24.248 | 62.582 | 1.00 31.96 | 6 |
| | | 16.373 | 23.539 | 63.246 | 1.00 34.84 | |
| ATOM | 1741 N ILE A 220 | 16.952 | 25.556 | | 1.00 34.04 | 8 |
| MOTA | 1742 CA ILE A 220 | | | 62.472 | 1.00 32.96 | 7 |
| ATOM | 1743 CB ILE A 220 | 15.826 | 26.196 | 63.129 | 1.00 32.50 | 6 |
| | 1744 CD 1LE A 220 | 16.259 | 27.037 | 64.350 | 1.00 32.32 | |
| MOTA | 1744 CG2 ILE A 220 | 15.029 | 27.644 | | 1.00 32.32 | 6 |
| ATOM | 1745 CG1 ILE A 220 | | 27.044 | 65.014 | 1.00 29.46 | 6 |
| MOTA | 1746 CD1 ILE A 220 | 16.978 | 26.160 | 65.374 | 1.00 29.65 | 6 |
| | 1747 C TE A 220 | 16.080 | 25.138 | 66.027 | 1.00 28.65 | |
| ATOM | 1747 C ILE A 220 | 15.140 | 27.106 | | 1.00 28.65 | 6 |
| MOTA | 1748 O ILE A 220 | | 27.100 | 62.123 | 1.00 35.36 | 6 |
| ATOM | 1749 N PRO A 221 | 15.469 | 28.290 | 62.009 | 1.00 35.52 | 8 |
| ATOM | 11 221 | 14.185 | 26.553 | 61.359 | 1.00 36.87 | |
| | 1750 CD PRO A 221 . | 13.718 | 25.158 | | 1.00 30.87 | 7 |
| ATOM | 1751 CA PRO A 221 | 13.445 | | 61.359 | 1.00 35.12 | 6 |
| ATOM | 1752 CB PRO A 221 | | 27.318 | 60.356 | 1.00 35.41 | 6 |
| ATOM | | 12.509 | 26.262 | 59.767 | 1.00 35.68 | 6 |
| | | 13.319 | 24.992 | 59.911 | 1 00 33.00 | |
| ATOM | 1754 C PRO A 221 | 12.696 | | | 1.00 33.86 | 6 |
| ATOM | 1755 O PRO A 221 | | 28.437 | 61.053 | 1.00 34.37 | 6 |
| ATOM | | 12.014 | 28.199 | 62.043 | 1.00 38.79 | 8 |
| | 222 | 12.815 | 29.655 | | | |
| ATOM | 1757 CA LEU A 222 | 12.138 | 30.796 | | 1.00 34.76 | 7 |
| ATOM | 1758 CB LEU A 222 | | | 61.166 | 1.00 33.87 | 6 |
| MOTA | 1759 CG LEU A 222 | 13.173 | 31.735 | 61.798 | 1.00 35.13 | 6 |
| | 1755 CG LEU A 222 | 14.104 | 31.163 | 62.876 | 1.00 33.07 | |
| ATOM | 1760 CD1 LEU A 222 | 15.234 | 32.150 | | 1.00 33.07 | 6 |
| ATOM | 1761 CD2 LEU A 222 | | | 63.154 | 1.00 34.04 | 6 |
| ATOM | 1762 C LEU A 222 | 13.312 | 30.856 | 64.141 | 1.00 32.39 | 6 |
| | | 11.287 | 31.567 | 60.157 | 1.00 32.15 | |
| ATOM | 1763 O LEU A 222 | 11.669 | 31.740 | | 1 . 3 | 6 |
| ATOM | 1764 N PRO A 223 | 10.127 | | 59.000 | 1.'0 31.32 | - 8 |
| MOTA | 1765 CD PRO A 223 | | 32.060 | 60.601 | 1.17 30.97 | 7 |
| | | 9.606 | 31.913 | | 1.00 32.34 | |
| Mota | 1766 CA PRO A 223 | | | | 1 00 32.34 | 6 |
| ATOM | 1767 CB PRO A 223 | 7 057 | | 33.769 | 1.00 30.55 | 6 |
| ATOM | | 7.957 | 32.893 | 60.702 | 1.00 29.44 | 6 |
| | | 8.626 | | | 1.00 31.02 | |
| ATOM | 1769 C PRO A 223 | | | EO 366 1 | 31.02 | 6 |
| ATOM | 1770 O PRO A 223 | | | 59.366 1 | 1.00 29.20 | 6 |
| ATOM | | | | 59.796 1 | 1.00 31.95 | 8 |
| | | 8.841 | | | 00 26.14 | |
| atom | 1772 CA LYS A 224 | ` | | 50 025 1 | 00 20.14 | 7 |
| MOTA | 1773 CB LYS A 224 | | 36.172 | 8.026 1 | .00 23.54 | 6 |
| | | 8.285 | 36.443 | 56.766 1 | .00 24:71 | 6 |
| | | 8.563 | 35.500 | 55.619 1 | .00 23.83 | |
| | 1775 CD LYS A 224 | | | 4 304 1 | 00 20.83 | 6 |
| ATOM | 1776 CE LYS A 224 | | | 4.394 1 | .00 20.59 | 6 |
| | | | 34.769 | 3.329 1 | .00 27.03 | 6 |
| | | 7.198 3 | 4.849 5 | 2.122 1 | .00 30.48 | |
| | 1778 C LYS A 224 | | 7.151 5 | | 00 00 | 7 |
| ATCM | 1779 O LYS A 224 | | | 9.111 1 | .00 25.48 | 6 |
| | | | 6.780 6 | 0.055 1 | .00 22.67 | 8 |
| | | 9.124 3 | | 8.960 1 | .00 26.88 | |
| | 1781 CA GLY A 225 | | | 0 025 1 | 00 20.00 | 7 |
| ATOM | 1782 C GLY A 225 | | | 9.925 1 | .00 29.80 | 6 |
| | | 3.330 3 | 9.188 6 | 1.286 1 | .00 32.96 | 6 |
| • | | | - | | | |

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| | 1702 | ^ | GLY A | 225 | 9.068 | 39.861 | 62.271 | 1.00 31.20 | 8 |
|--------------|--------------|-----|--------|-----|--------|--------|---------|-------------|-----|
| MOTA | 1783 | 0 | | | | | 61.338 | 1.00 32.86 | 7 |
| MOTA | 1784 | N | LEU A | | 10.299 | 38.216 | | 1.00 34.55 | 6 |
| MOTA | 1785 | CA | LEU A | | 10.975 | 37.877 | 62.575 | | |
| ATOM | 1786 | CB | LEU A | | 12.149 | 36.958 | 62.255 | 1.00 34.46 | 6 |
| MOTA | 1787 | CG | LEU A | | 12.982 | 36.413 | 63.407 | 1.00 34.48 | 6 |
| ATOM | 1788 | | LEU A | | 12.146 | 35.425 | 64.212 | 1.00 33.18 | 6 |
| ATOM | 1789 | CD2 | LEU A | 226 | 14.207 | 35.724 | 62.847 | 1.00 31.39 | 6 |
| MOTA | 1790 | С | LEU A | | 11.481 | 39.160 | 63.255 | 1.00 36.29 | 6 |
| ATOM | 1791 | 0 | LEU A | 226 | 12.156 | 39.970 | 62.613 | 1.00 33.87 | 8 |
| ATOM | 1792 | N | ASN A | | 11.131 | 39.358 | 64.531 | 1.00 37.31 | 7 |
| MOTA | 1793 | CA | ASN A | | 11.592 | 40.536 | 65.279 | 1.00 37.26 | 6 |
| | 1794 | СВ | ASN A | | 10.444 | 41.212 | 66.053 | 1.00 35.57 | 6 |
| ATOM | 1795 | CG | ASN A | | 9.920 | 40.368 | 67.208 | 1.00 36.07 | 6 |
| ATOM | | OD1 | | | 10.678 | 39.940 | 68.089 | 1.00 35.08 | 8 |
| ATOM | 1796 | | | | 8.611 | 40.143 | 67.218 | 1.00 32.33 | 7 |
| ATOM | 1797 | ND2 | ASN A | | 12.688 | 40.096 | 66.259 | 1.00 37.95 | 6 |
| ATOM | 1798 | C | ASN A | | | | 66.473 | 1.00 37.08 | .8 |
| ATOM | 1799 | 0 | ASN A | | 12.869 | 38.890 | | 1.00 36.07 | 7 |
| ATOM | 1800 | N | ASP A | | 13.403 | 41.063 | 66.832 | | 6 |
| ATOM | 1801 | CA | ASP A | | 14.505 | 40.754 | 67.751 | 1.00 37.63 | |
| ATOM | 1802 | CB | ASP A | | 14.996 | 42.007 | 68.486 | 1.00 36.48 | |
| ATOM | 1803 | CG | ASP A | | 15.480 | 43.088 | 67.545 | 1.00 37.52 | 6 |
| ATOM | 1804 | | ASP A | | 15.936 | 42.752 | 66.427 | 1.00 35.28 | 8 |
| ATOM | 1805 | OD2 | ASP A | | 15.426 | 44.274 | 67.937 | 1.00 39.01 | 8 |
| ATOM | 1806 | С | ASP A | 228 | 14.204 | 39.678 | 68.783 | 1.00 37.56 | 6 |
| MOTA | 1807 | 0 | ASP A | | 14.921 | 38.678 | 68.869 | 1.00 39.53 | 8 |
| ATOM | 1808 | N | ASN A | | 13.155 | 39.889 | 69.572 | 1.00 38.37 | 7 |
| ATOM | 1809 | CA | ASN A | 229 | 12.766 | 38.935 | 70.605 | 1.00 37.49 | 6 |
| ATOM | 1810 | CB | ASN A | 229 | 11.422 | 39.352 | 71.200 | 1.00 37.38 | 6 |
| ATOM | 1811 | CG | ASN A | 229 | 11.490 | 40.709 | 71.877 | 1.00 40.47 | 6 |
| ATOM | 1812 | OD1 | ASN A | 229 | 12.041 | 40.840 | 72.973 | 1.00 41.76 | 8 |
| ATOM | 1813 | ND2 | ASN A | 229 | 10.960 | 41.735 | 71.212 | 1.00 36.50 | 7 |
| ATOM | 1814 | С | ASN A | 229 | 12.680 | 37.530 | 70.017 | 1.00 37.64 | 6 |
| ATOM | 1815 | 0 | ASN A | 229 | 13.446 | 36.634 | 70.395 | 1.00 35.76 | - 8 |
| ATOM | 1816 | N | GLU A | | 11.758 | 37.351 | 69.076 | 1.00 36.01 | 7 |
| ATOM | 1817 | CA | GLU A | | 11.574 | 36.062 | 68.425 | 1.00 34.74 | 6 |
| ATOM | 1818 | CB | GLU A | | 10.753 | 36.242 | 67.153 | 1.00 35.55 | 6 |
| ATOM | 1819 | CG | GLU A | | 9.382 | 36.820 | 67.407 | 1.00 36.95 | 6 |
| ATOM | 1820 | CD | GLU A | | 8.580 | 36.960 | 66.144 | 1.00 35.30 | 6 |
| ATOM | 1821 | | GLU A | | 9.042 | 37.670 | 65.229 | 1.00 36.98 | 8 |
| ATOM | 1822 | OE2 | GLU A | | 7.490 | 36.361 | 66.065 | 1.00 36.71 | 8 |
| ATOM | 1823 | c | GLU A | | 12.916 | 35.421 | 68.082 | 1.00 33.92 | 6 |
| ATOM | 1824 | ō | GLU A | | 13.143 | 34.238 | 68.346 | 1.00 32.74 | 8 |
| | 1825 | N | PHE A | | 13.804 | 36.207 | 67.487 | 1.00 32.03 | 7 |
| ATOM ATOM | 1826 | CA | PHE A | | 15.116 | 35.712 | 67.123. | 1.00 30.55 | 6 |
| | 1827 | CB | PHE A | | 15.932 | 36.821 | 66.460 | 1.00 33.86 | 6 |
| MOTA MOTA | 1828 | CG | HE A | | 17.295 | 36.381 | 66.012 | 1.00 36.97 | ` 6 |
| | 1829 | | `_HE A | | 17.438 | 35.334 | 65.102 | 1.00 40.41 | 6 |
| MOTA | 1830 | | HE A | | 18.436 | 37.021 | 66.480 | 1.00 36.58 | 6 |
| ATOM | 1831 | CEI | PHE A | 231 | 18.709 | 34.932 | 64.661 | 1.00 43.00 | 6 |
| MOTA | | | PHE A | | 19.711 | 36.632 | 66.049 | 1.00 39.07 | 6 |
| MOTA | 1832 1833 | | PHE A | | 19.849 | 35.586 | 65.137 | 1.00 40.52 | 6 |
| ATOM | | | PHE A | | 15.835 | 35.232 | 68.376 | .1.00 30.63 | 6 |
| ATOM | 1834 | C | PHE A | 231 | 16.177 | 34.042 | 68.497 | 1.00 29.66 | 8 |
| ATOM | 1835 | 0 | PHE A | | 16.049 | | | 1.00 24.94 | 7 |
| ATOM | 1836 | N | LEU A | | | 36.162 | 70.556 | 1.00 22.82 | 6 |
| ATOM | 1837 | CA | LEU A | 232 | 16.742 | 35.857 | | 1.00 24.96 | . 6 |
| ATOM | 1838 | CB | LEU A | | 16.724 | 37.084 | 71.468 | 1.00 29.34 | 6 |
| MOTA | 1839 | CG | LEU A | | 17.507 | 38.282 | 70.890 | 1.00 24.38 | 6 |
| ATOM | 1840 | CD1 | LEU A | | 17.316 | 39.549 | 71.746 | | 6 |
| MOTA | 1841 | | LEU A | | 18.991 | 37.903 | 70.787 | 1.00 27.39 | 6 |
| MOTA | 1842 | С | LEU A | | 16.150 | 34.638 | 71.261 | 1.00 22.44 | 8 |
| ATOM | 1843 | 0 | LEU A | | 16.882 | 33.793 | 71.767 | 1.00 20.37 | |
| MOTA | 1844 | N | PHE A | | 14.825 | 34.552 | 71.289 | 1.00 24.81 | 7 |
| MOTA | 1845 | CA | PHE A | | 14.131 | 33.422 | 71.905 | 1.00 25.81 | 6 |
| ATOM | 1845 | CB | PHE A | 233 | 12.623 | 33.535 | 71.641 | 1.00 24.37 | 6 |
| ATOM | 1847 | CG | PHE A | 233 | 11.811 | 32.373 | 72.157 | 1.00 24.18 | 6 |
| MOTA | 1848 | | PHE A | 233 | 11.491 | 32.264 | 73.503 | 1.00 25.59 | 6 |

| ATOM 1849 CD2 PHE A 233 | 11 |
|--------------------------|---|
| ATOM 1850 CE1 PHE A 233 | 11.339 31.397 71.284 1.00 25.75 |
| ATOM 1851 CE2 PHE A 233 | ±0.030 31.198 73 974 1 00 5c cc |
| THE R 233 | 10.548 30.327 71 747 1 00 25.55 |
| | 10.228 30.232 73 097 1 00 20 |
| 1 III A 233 | 14 662 |
| FIE A 233 | 15 004 71 1100 20.04 |
| ATOM 1855 N ALA A 234 | 14 504 11 11 11 11 11 11 11 11 11 11 11 11 11 |
| ATOM 1856 CA ALA A 234 | 15 000 32.08/ 69.949 1.00 27.27 |
| ATOM 1857 CB ALA A 234 | 14.707 30.921 69.209 1.00 30.24 |
| ATOM 1858 C ALA A 234 | +3·/2/ 31-10/ 67 720 1 00 22 1 |
| ATOM 1859 O ALA A 234 | 10.303 30.645 69.433 1 nn 3n 7c |
| | 16.981 29.491 69.488 1 00 30 04 |
| | 17.363 31.695 69 563 1.00 35.04 |
| C. DEO R 233 | 18.789 31.486 69.700 1.00 31.84 7 |
| CE LLU K 233 | 10 540 55 55 55 55 55 55 55 55 55 55 55 55 55 |
| ATOM 1863 CG LEU A 235 | 21 020 |
| ATOM 1864 CD1 LEU A 235 | 21 625 2 6 |
| ATOM 1865 CD2 LEU A 235 | 31 203 34.136 69.205 1.00 36.44 6 |
| ATOM 1866 C LEU A 235 | 21.803 31.939 70.330 1.00 35 64 6 |
| ATOM 1867 O LEU A 235 | 10.370 30.846 71.176 1.00 30 75 E |
| ATOM 1868 N GLU A 236 | ~~···································· |
| 5 5D0 A 236 | 18.347 31 435 72 102 1 00 22 |
| 3 GLU A 236 | 18.418 30.931 73 561 1 00 22 22 |
| 02 GDU A 236 | 17.479 31 730 74 452 1.00 33.32 6 |
| - 00 G20 A 236 | 17.843 33 176 74 675 1.00 33.06 6 |
| ATOM 1872 CD GLU A 236 | 16 610 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 |
| ATOM 1873 OE1 GLU A 236 | 15 606 22 2.040 1.00 47.12 6 |
| ATOM 1874 OE2 GLU A 236 | 16 570 - 5 5 5 5 5 5 6 7 8 |
| ATOM 1875 C GLU A 236 | 17 000 33.130 74.297 1.00 49.07 8 |
| ATOM 1876 O GLU A 236 | 10.715 29.4/3 73.639 1.00 34.65 6 |
| ATOM 1877 N LYS A 237 | 10.715 28.593 74.116 1.00 30 43 |
| ATOM 1878 CA LYS A 237 | 10.767 29.250 73.176 1 00 36 67 |
| ATOM 1879 CB LYS A 237 | 16.138 27.943 73.175 1.00 35 51 |
| ATOM 1880 CG LYS A 237 | 14.731 28.060 72.452 1.00 37 01 6 |
| DID R 23/ | 13.745 27.032 72 848 1 00 20 65 |
| | 12.712 27.605 73 821 1 00 40 66 |
| | 13.312 28.054 75 153 1.00 40.66 6 |
| 213 A 23/ | 10 250 20 10 10 10 10 40 38 6 |
| ATOM 1884 C LYS A 237 | 17 000 7 |
| ATOM 1885 O LYS A 237 | 17 315 35 100 33.07 6 |
| ATOM 1886 N SER A 238 | 17 455 22 10.001 1.00 30.60 8 |
| ATOM 1887 CA SER A 238 | 10 270 25 1.00 33.59 / |
| ATOM 1888 CB SER A 238 | 10 450 |
| ATOM 1889 OG SER A 238 | 10 014 1.00 32.01 6 |
| ATOM 1890 C SER A 238 | 10.650 28.168 69.075 1.00 37.80 8 |
| ATOM 1891 O SER A 238 | 13.030 25.928 71.032 1.00 31.94 6 |
| ATOM 1892 N LEU A 239 | 20.064 24.758 70.990 1.00 26 88 9 |
| ATOM 1893 CA LEU A 239 | 20.337 26.920 71.564 1.00 31 19 7 |
| ATOM 1894 CB LEU A 239 | 41.660 26.650 72 147 1 00 20 00 |
| <u> </u> | 44.433 47.914 77 770 1 00 20 02 |
| | 22.650 29.087 71 817 1 00 24 21 |
| A Z J J | 23.210 30 189 72 605 1 00 24.31 |
| 233 | 22 24 23 |
| ATOM 1898 C LEU A 239 | 23 462 23.11 6 |
| ATOM 1899 O LEU A 239 | 22 270 24 250 75.275 1.00 31.99 6 |
| ATOM 1900 N GLU A 240 | 20 20 |
| ATOM 1901 CA GLU A 240 | 20 00. |
| ATOM 1902 CB GLU A 240 | 10 700 15.150 1.00 38,61 6 |
| ATOM 1903 CG GLU A 240 | 10.799 25.369 75.842 1.00 43.21 6 |
| ATOM 1904 CD GLU A 240 | 10.300 24.468 77.045 1.00 53 52 6 |
| ATOM 1905 OE1 GLU A 240 | 13.07/ 24.383 78.022 1.00 56.39 6 |
| ATOM 1906 OE2 GLU A 240 | 19.969 25.399 78.701 1.00 57.81 8 |
| ATOM 1907 C GLU A 240 | 20.318 23.304 78.093 1.00 55 12 8 |
| | 20.033 23.507 74.722 1.00 30 32 |
| | 30 530 |
| ATOM 1909 N ILE A 241 | 10 405 |
| TOM 1910 CA ILE A 241 | 10 310 -0.232 /3.30/ 1.00 40.74 7 |
| TOM 1911 CB ILE A 241 | 10 45" -1.050 15.055 1.00 38.08 6 |
| TCM · 1912 CG2 ILE A 241 | 10 575 |
| TOM 1913 CG1 ILE A 241 | 17 010 =0.500 /1.000 1.00 31.39 6 |
| TOM 1914 CD1 ILE A 241 | 17.012 22.226 72.056 1.00 31.06 6 |
| | 16.147 22.478 70.843 1.00 27.53 6 |
| | • |

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| | | | | • | | | | | |
|--------|------|-----|--------|-------|--------|--------|-----------------|------------|-----|
| MOTA | 1915 | С | ILE A | 241 | 20.713 | 21,372 | 72.747 | 1.00 39.56 | 6 |
| ATOM | 1916 | 0 | ILE A | | 20.984 | 20.189 | 72.936 | 1.00 40.82 | 8 |
| | 1917 | N | VAL A | | 21.605 | 22.254 | 72.299 | 1.00 41.93 | 7 |
| ATOM | | | | | | 21.842 | 72.015 | 1.00 45.09 | 6 |
| MOTA | 1918 | CA | VAL A | | 22.979 | | | | |
| ATOM | 1919 | CB | VAL A | | 23.808 | 22.959 | 71.329 | 1.00 45.76 | 6 |
| ATOM | 1920 | CG1 | VAL A | | 25.242 | 22.479 | 71.116 | 1.00 43.09 | 6 |
| ATOM | 1921 | CG2 | VAL A | 242 | 23.182 | 23.334 | 69.991 | 1.00 46.41 | 6 |
| ATOM | 1922 | С | VAL A | 242 | 23.698 | 21.453 | 73.300 | 1.00 45.69 | 6 |
| | 1923 | ō | VAL A | | 24.191 | 20.331 | 73.423 | 1.00 46.30 | 8 |
| ATOM | | | LYS A | | 23.750 | 22.373 | 74.259 | 1.00 44.60 | 7 |
| ATOM | 1924 | N | | | | | 75.513 | 1.00 46.96 | 6 |
| ATOM | 1925 | CA | LYS A | | 24.427 | 22.088 | | | |
| ATOM | 1926 | CB | LYS A | . 243 | 24.214 | 23.217 | 76.527 | 1.00 49.49 | 6 |
| MOTA | 1927 | CG | LYS A | 243 | 25.061 | 23.023 | 77.795 | 1.00 54.90 | 6 |
| MOTA | 1928 | CD | LYS A | 243 | 24.652 | 23.934 | 78.939 | 1.00 58.95 | 6 |
| ATOM | 1929 | CE | LYS A | 243 | 24.782 | 25.399 | 78.57 7 | 1.00 64.13 | 6 |
| ATOM | 1930 | NZ | LYS A | | 24.274 | 26.283 | 79.676 | 1.00 66.93 | 7 |
| | | C | LYS A | | 23.965 | 20.767 | 76.135 | 1.00 47.06 | 6 |
| MOTA | 1931 | | | | | 20.707 | 76.845 | 1.00 46.39 | 8 |
| MOTA | 1932 | 0 | LYS A | | 24.735 | | | | 7 |
| MOTA | 1933 | И | GLU A | | 22.716 | 20.380 | 75.878 | 1.00 47.51 | |
| ATOM | 1934 | CA | GLU A | 244 | 22.172 | 19.136 | 76.429 | 1.00 51.33 | ` 6 |
| ATOM | 1935 | CB | GLU A | 244 | 20.650 | 19.061 | 76.259 | 1.00 54.49 | 6 |
| ATOM | 1936 | CG | GLU A | 244 | 19.843 | 20.199 | 76.842 | 1.00 62.61 | 6 |
| ATOM | 1937 | CD | GLU A | 244 | 18.360 | 20.089 | 76.489 | 1.00 65.15 | 6 |
| | 1938 | | GLU A | | 17.572 | 20.980 | 76.888 | 1.00 66.49 | 8 |
| MOTA | | OE2 | GLU A | | 17.986 | 19.108 | 75.807 | 1.00 64.82 | 8 |
| ATOM | 1939 | | | | | 17.936 | 75.698 | 1.00 50.17 | 6 |
| ATOM | 1940 | C | GLU A | | 22.745 | | | 1.00 51.54 | 8 |
| MOTA | 1941 | 0 | GLU A | | 22.866 | 16.846 | 76.259 | | |
| MOTA | 1942 | N | VAL A | 245 | 23.104 | 18.148 | 74.441 | 1.00 47.70 | 7 |
| ATOM | 1943 | CA | VAL A | 245 | 23.587 | 17.063 | 73.611 | 1.00 45.43 | 6 |
| ATOM | 1944 | CB | VAL A | 245 | 22.704 | 16.980 | 72.336 | 1.00 48.47 | 6 |
| ATOM | 1945 | CG1 | VAL A | 245 | 23.082 | 15.765 | 71.499 | 1.00 51.87 | 6 |
| | 1946 | CG2 | | | 21.226 | 16.934 | 72.731 | 1.00 45.65 | 6 |
| ATOM | - | C | VAL A | | 25.056 | 17.070 | 73.185 | 1.00 43.01 | ·6 |
| ATOM | 1947 | | | | | 16.005 | 72.946 | 1.00 39.28 | 8 |
| ATOM | 1948 | 0 | VAL A | | 25.620 | | | 1.00 40.53 | 7 |
| ATOM . | 1949 | N | PHE A | | 25.682 | 18.245 | 73.109 | | 6 |
| ATOM | 1950 | CA | PHE A | | 27.063 | 18.321 | 72.633 | 1.00 38.56 | |
| MOTA | 1951 | CB | PHE A | 246 | 27.023 | 18.700 | 71.154 | 1.00 36.85 | 6 |
| ATOM | 1952 | CG | PHE A | 246 | 28.315 | 18.487 | 70.415 | 1.00 36.46 | 6 |
| ATOM | 1953 | CD1 | PHE A | 246 | 28.749 | 17.201 | 70.098 | 1.00 32.95 | 6 |
| ATOM | 1954 | CD2 | PHE A | | 29.064 | 19.582 | 69.967 | 1.00 35.51 | 6 |
| | 1955 | CE1 | PHE A | | 29.903 | 17.004 | 69.337 | 1.00 33.80 | 6 |
| ATOM | | CE2 | PHE A | | 30.222 | 19.397 | 69.206 | 1.00 34.46 | 6 |
| MOTA | 1956 | | | | 30.640 | 18.103 | 68.889 | 1.00 35.54 | 6 |
| ATOM | 1957 | cz | PHE A | | | | 73.371 | 1.00 40.83 | 6 |
| ATOM | 1958 | С | PHE A | _ | 27.970 | 19.311 | | | 8 |
| MOTA | 1959 | 0 | PHE A | 246 | 27.613 | 20.478 | 73.549 | 1.00 40.32 | |
| ATOM | 1960 | N | GLU A | 247 | 29.141 | 18.839 | 73.802 | 1.00 42.54 | 7 |
| ATOM | 1961 | CA | GLU A | 247 | 30.128 | 19.695 | 74.467 | 1.00 43.93 | 6 |
| ATOM | 1962 | CB | GLU A | 247 | 30.655 | 19.075 | 75. 77 0 | 1.00 45.67 | 6 |
| ATOM | 1963 | CG | GLU A | | 29.763 | 19.243 | 77.005 | 1.00 51.63 | 6 |
| | 1964 | CD | GLU A | | 28.478 | 18.424 | 76.962 | 1.00 57.42 | 6 |
| ATOM | | | | | | 18.644 | 76.058 | 1.00 62.12 | 8 |
| MOTA | 1965 | OE1 | GLU A | | 27.645 | | 77.845 | 1.00 59.43 | 8 |
| MOTA | 1966 | | GLU A | 44/ | 28.296 | 17.557 | | 1.00 43.62 | 6 |
| ATOM | 1967 | С | GLU A | | 31.268 | 19.839 | 73.464 | | |
| · MOTA | 1968 | 0 | GLU A | | 32.077 | 18.931 | 73.294 | 1.00 44.25 | 8 |
| ATOM | 1969 | N | PRO A | 248 | 31.342 | 20.988 | 72.780 | 1.00 43.65 | 7 |
| ATOM | 1970 | CD | PRO, A | | 30.439 | 22.143 | 72.863 | 1.00 42.73 | 6 |
| | 1971 | CA | PRO A | | 32.371 | 21.260 | 71.779 | 1.00 43.28 | 6 |
| ATOM | | | PRO A | 248 | 31.802 | 22.480 | 71.042 | 1.00 43.03 | 6 |
| ATOM | 1972 | CB | PRO A | 240 | | 22.474 | 71.415 | 1.00 43.02 | 6 |
| ATOM | 1973 | CG | PRO A | 240 | 30.317 | | | 1.00 43.37 | 6 |
| ATOM | 1974 | С | PRO A | 248 | 33.759 | 21.552 | 72.331 | | |
| ATOM | 1975 | 0 | PRO A | 248 | 33.896 | 22.286 | 73.305 | 1.00 45.44 | 8 |
| ATOM | 1976 | N | GLU A | | 34.788 | 20.982 | 71.710 | 1.00 42.38 | 7 |
| | 1977 | CA | GLU A | | 36.151 | 21.263 | 72.136 | 1.00 41.56 | 6 |
| ATOM | - | CB | GLU A | 249 | 37.148 | 20.275 | 71.528 | 1.00 42.06 | 6 |
| ATOM | 1978 | | | | 36.935 | 18.816 | 71.887 | 1.00 44.28 | 6 |
| ATOM | 1979 | CG | GLU A | | | | 71.295 | 1.00 44.79 | 6 |
| ATOM | 1980 | CD | GLU A | | 38.015 | 17.908 | 11.433 | 1.00 33.73 | • |
| | | • | | • • • | | | | | |
| | | | | | | | | | |

| ATOM | 1 1981 OE1 GLU A 249 | 38.208 17.938 70.054 1.00 42.47 8 |
|--------------|--|--|
| ATOM | | 38.666 17.168 72.072 1 00 39 73 |
| ATOM | | 36.443 22.654 71.583 1.00 40.99 6 |
| ATOM | | 37.150 23.450 72.204 1.00 42.83 8 |
| ATOM | | 35.879 22.936 70.407 1.00 37.65 7 |
| ATOM ATOM | | 36.059 24.221 69.728 1.00 34.87 6 |
| ATOM | | 37.294 24.203 68.789 1.00 34.53 6 |
| ATOM | | 37.129 23.113 67.728 1.00 32.76 6 |
| ATOM | | 37.487 25.581 68.144 1.00 29.62 6 |
| ATOM | | 34.830 24.527 68.891 1.00 32.67 6 |
| MOTA | | 34.162 23.610 68.421 1.00 33.96 8 34.539 25.810 68.690 1.00 29.71 7 |
| ATOM | | 27 260 06 100 25.71 |
| ATOM | | 22 105 25 151 |
| MOTA | | |
| ATOM | | 71 557 20 002 50 500 |
| MOTA | 1997 CE1 TYR A 251 | 31 430 30 105 50 105 |
| ATOM | 1998 CD2 TYR A 251 | 22 454 65 454 |
| MOTA | 1999 CE2 TYR A 251 | 32.494 28.181 70.696 1.00 30.20 6 32.384 29.477 71.193 1.00 33.89 6 |
| MOTA | 2000 CZ TYR A 251 | 31.854 30.482 70.391 1.00 34.75 6 |
| MOTA | | 31.743 31.773 70.867 1.00 33.52 8 |
| ATOM | 2002 C TYR A 251 | 33.570 27.384 66.992 1.00 27.48 6 |
| ATOM | 2003 O TYR A 251 | 34.167 28.402 67.366 1.00 24.78 8 |
| ATOM | 2004 N LEU A 252 | 33.063 27.254 65.773 1.00 24.80 7 |
| ATOM | 2005 CA LEU A 252 | 33.150 28.332 64.815 1.00 23.40 6 |
| ATOM. | 2006 CB LEU A 252 | 33.631 27.810 63.451 1.00 21.32 6 |
| ATOM | 2007 CG LEU A 252 2008 CD1 LEU A 252 | 35.126 27.456 63.385 1.00 21.84 6 |
| MOTA MOTA | 2008 CD1 LEU A 252 2009 CD2 LEU A 252 | 35.457 26.373 64.395 1.00 22.51 6 |
| ATOM | 2010 C LEU A 252 | 35.499 26.999 61.986 1.00 22.07 6 |
| ATOM | 2011 O LEU A 252 | 31.762 28.959 64.729 1.00 22.56 6 |
| ATOM | 2012 N LEU A 253 | 30.750 28.266 64.856 1.00 21.99 8 31.734 30.277 64.554 1.00 21.01 7 |
| ATOM | 2013 CA LEU A 253 | 7.00 21.01 |
| ATOM | 2014 CB LEU A 253 | 30 353 31 011 |
| ATOM | 2015 CG LEU A 253 | 29.198 32.942 65.842 1.00 21.61 6 |
| ATOM | 2016 CD1 LEU A 253 | 27.849 32.220 65.860 1.00 22.23 6 |
| MOTA | 2017 CD2 LEU A 253 | 29.395 33.716 67.145 1.00 22.90 6 |
| MOTA | 2018 C LEU A 253 | 30.539 31.901 63.198 1.00 20.05 6 |
| ATOM | 2019 O LEU A 253 | 31.466 32.691 62.987 1.00 18.17 8 |
| ATOM | 2020 N GLN A 254 | 29.544 31.720 62.340 1.00 19.40 7 |
| ATOM | 2021 CA GLN A 254 | 29.488 32.490 61.115 1.00 18.17 6 |
| MOTA | 2022 CB GLN A 254 2023 CG GLN A 254 | 29.017 31.592 59.969 1.00 9.67 6 |
| ATOM ATOM | 2023 CG GLN A 254 2024 CD GLN A 254 | 27.584 31.713 59.601 1.00 18.43 6 |
| ATOM | 2025 OE1 GLN A 254 | 27.368 32.766 58.549 1.00 19.97 6 |
| ATOM | 2026 NE2 GLN A 254 | 27.917 32.677 57.450 1.00 22.54 8 26.564 33.769 58.869 1.00 22.89 7 |
| ATOM | 2027 C GLN A 254 | 2.00 22.00 |
| ATOM | 2028 O GLN A 254 | 77 470 98 445 46 44 |
| MOTA | 2029 N LEU A 255 | 27.470 33.415 62.060 1.00 18.77 8 28.905 34.854 61.067 1.00 23.02 7 |
| ATOM | 2030 CA LEU A 255 | 28.132 36.052 61.369 1.00 23.77 6 |
| ATOM | 2031 CB LEU A 255 | 28.963 36.993 62.242 1.00 26.84 6 |
| MOTA | 2032 CG LEU A 255 | 29.226 36.556 63.684 1.00 29.34 6 |
| MOTA | 2033 CD1 LEU A 255 | 30.196 37.520 64.331 1.00 30.65 6 |
| ATOM | 2034 CD2 LEU A 255 | 27.902 36.506 64.456 1.00 28.42 6 |
| MOTA | 2035 C LEU A 255 | 27.605 36.842 60.197 1.00 24.84 6 |
| MOTA | 2036 O LEU A 255 | 27.774 38.066 60.149 1.00 24.94 8 |
| MOTA | 2037 N GLY A 256 | 26.969 36.158 59.254 1.00 25.07 7 |
| ATOM | 2038 CA GLY A 256 | 26.408 36.858 58.117 1.00 26.11 6 |
| MOTA | 2039 C GLY A 256 | 25.506 37.956 58.644 1.00 27.11 6 |
| ATOM | 2040 O GLY A 256 2041 N THR A 257 | 24.742 37.734 59.584 1.00 25.67 8 |
| ATOM ATOM | 2041 N THR A 257 2042 CA THR A 257 | 25.599 39.150 58.072 1.00 27.85 7 |
| ATOM | 2043 CB THR A 257 | 24.757 40.244 58.536 1.00 29.28 6 25.517 41.597 58.545 1.00 27.98 6 |
| ATOM | 2344 OG1 THR A 257 | |
| ATOM | 2045 CG2 THR A 257 | |
| MOTA | 2046 C THR A 257 | 26.686 41.541 59.510 1.00 26:45 6 23.477 40.392 57.722 1.00 28.39 6 |
| | · | 10.332 31.122 1.00 40.39 B |

| ATOM | 2047 | 0 | THR . | A 257 | | 22.747 | 41.370 | 57.879 | 1.00 29.49 | 8 |
|--------|------|-----|---------|-------|---|--------|---------------------|---------|------------|-----|
| ATOM | 2048 | N | ASP . | A 258 | | 23.192 | 39.414 | 56.867 | 1.00 29.13 | |
| MOTA | 2049 | | _ | A 258 | | 21.977 | 39.471 | 56.065 | 1.00 30.49 | • |
| MOTA | 2050 | | | A 258 | | 22.004 | 38.432 | 54.933 | 1.00 28.22 | - |
| ATOM | 2051 | . – | | A 258 | | 22.337 | 37.033 | 55.416 | 1.00 29.39 | _ |
| ATOM | 2052 | | 1 ASP | | | 21.893 | 36.653 | 56.520 | 1.00 30.16 | |
| ATOM | 2053 | | 2 ASP | | | 23.019 | 36.292 | 54.667 | 1.00 29.97 | - |
| ATOM | 2054 | | - | A 258 | | 20.646 | 39.355 | 56.826 | 1.00 30.50 | _ |
| ATOM | 2055 | | | A 258 | | 19.601 | 39.622 | 56.248 | 1.00 32.87 | _ |
| ATOM | 2056 | | | A 259 | | 20.650 | 38.912 | 58.101 | 1.00 32.87 | _ |
| ATOM | 2057 | | | A 259 | | 21.711 | | | | |
| | | | | A 259 | • | | 38.338 | 58.952 | 1.00 33.56 | - |
| MOTA | 2058 | | | A 259 | | 19.366 | 38.821 | 58.806 | 1.00 31.73 | _ |
| MOTA | 2059 | CB | | - | | 19.705 | 37.912 | 59.987 | 1.00 31.87 | |
| MOTA | 2060 | | | | | 21.067 | 38.373 | 60.333 | 1.00 31.73 | _ |
| ATOM | 2061 | C | | A 259 | | 18.817 | 40.184 | 59.260 | 1.00 30.86 | _ |
| MOTA | 2062 | 0 | PRO A | | | 17.736 | 40.270 | 59.84-5 | 1.00 29.78 | - |
| ATOM | 2063 | N | LEU A | | | 19.565 | 41.245 | 58.980 | 1.00 29.58 | |
| MOTA | 2064 | CA | LEU A | | | 19.161 | 42.592 | 59.375 | 1.00 29.15 | _ |
| MOTA | 2065 | CB | LEU A | | | 20.367 | 43.542 | 59.275 | 1.00 27.14 | _ |
| ATOM | 2066 | CG | LEU A | | | 21.543 | 43.286 | 60.234 | 1.00 22.17 | _ |
| ATOM | 2067 | | 1 LEU A | | | 22.794 | 43.919 | 59.684 | 1.00 15.79 | |
| MOTA | 2068 | | 2 LEU A | | | 21.211 | 43.793 | 61.633 | 1.00 16.25 | 6 |
| MOTA | 2069 | c | LEU A | | | 17.992 | 43.165 | 58.576 | 1.00 28.09 | - |
| ATOM | 2070 | 0 | LEU A | | | 17.787 | 42.834 | 57.410 | 1.00 29.61 | 8 |
| ATOM | 2071 | N | LEU A | | | 17.237 | 44.044 | 59.223 | 1.00 29.29 | |
| ATOM | 2072 | CA | LEU A | | | 16.097 | 44.693 | 58.596 | 1.00 29.71 | 6 |
| MOTA | 2073 | CB | LEU A | | | 15.540 | 45.788 | 59.513 | 1.00 29.62 | 6 |
| ATOM | 2074 | CG | LEU A | | | 14.406 | 46.664 | 58.950 | 1.00 28.14 | 6 |
| ATOM | 2075 | | L LEU A | | | 13.144 | 45.819 | 58.803 | 1.00 24.82 | 6 |
| MOTA | 2076 | | LEU A | | | 14.139 | 47.859 | 59.882 | 1.00 25.45 | |
| MOTA | 2077 | C | LEU- A | | | 16.461 | 45.322 | 57.259 | 1.00 29.50 | 6 |
| ATOM | 2078 | 0 | LEU A | | | 15.717 | 45.198 | 56.295 | 1.00 31.67 | 8 |
| ATOM | 2079 | N | GLU A | | | 17.603 | 45.998 | 57.201 | 1.00 31.54 | 7 |
| MOTA | 2080 | CA | | 262 . | | 18.015 | 46.664 | 55.973 | 1.00 31.93 | 6 |
| ATOM | 2081 | CB | GLU A | | | 19.049 | 47.758 | 56.279 | 1.00 29.34 | 6 |
| MOTA | 2082 | CG | GLU A | | | 18.496 | 48.931 | 57.086 | 1.00 28.52 | 6 |
| MOTA | 2083 | CD | GLU A | | | 18.449 | 48.687 | 58.589 | 1.00 29.76 | 6 |
| ATOM | 2084 | | GLU A | | | 18.175 | 47.548 | 59.029 | 1.00 30.12 | 8 |
| ATOM | 2085 | | GLU A | | | 18.661 | 49.661 | 59.338 | 1.00 27.69 | 8 |
| MOTA | 2086 | C | GLU A | | | 18.526 | 45.754 | 54.857 | 1.00 34.29 | 6 |
| ATOM | 2087 | 0 | GLU A | | | 18.690 | 46.199 | 53.722 | 1.00 35.20 | 8 |
| MOTA | 2088 | N | ASP A | | | 18.778 | 44.486 | 55.158 | 1.00 36.55 | 7 |
| ATOM | 2089 | CA | ASP A | | | 19.245 | 43.582 | 54.117 | 1.00 39.50 | 6 |
| MOTA | 2090 | CB | ASP A | | | 20.354 | 42.672 | 54.641 | 1.00 38.42 | 6 |
| ATOM | 2091 | CG | ASP A | | | 20.982 | 41.847 | 53.538 | 1.00 39.33 | 6 |
| ATOM | 2092 | | ASP A | | | 22.064 | 11.263 | 53.762 | 1.00 38.86 | 8 |
| ATOM | 2093 | OD2 | | | | 20.384 | 11.779 | 52.443 | 1.00 39.50 | 8 |
| ATOM | 2094 | C | ASP A | | | 18.046 | 2.775 | 53.634 | 1.00 42.83 | 6 |
| ATOM | 2095 | 0 | ASP A | | | 17.474 | 41.966 | 54.381 | 1.00 44.22 | 8 |
| ATOM | 2096 | N | TYR A | | | 17.673 | 43.002 | 52.377 | 1.00 44.14 | 7 |
| MOTA | 2097 | CA | TYR A | | | 16.508 | 42.357 | 51.796 | 1.00 46.67 | 6 |
| ATOM | 2098 | CB | TYR A | | | 16.031 | 43.149 | 50.568 | 1.00 54.61 | 6 |
| ATOM | 2099 | CG | TYR A | | | 16.824 | 42.939 | 49.294 | 1.00 63.02 | 6 |
| MOTA | 2100 | | TYR A | | | 16.510 | 41.897 [.] | 48.412 | 1.00 65.73 | 6 |
| MOTA | 2101 | CE1 | | | | 17.230 | 41.709 | 47.226 | 1.00 68.35 | . 6 |
| ATOM | 2102 | | TYR A | | | 17.882 | 43.786 | 48.962 | 1.00 66.23 | · б |
| MOTA | 2103 | CE2 | TYR A | 264 | | 18.611 | 43.606 | 47.780 | 1.00 68.63 | 6 |
| MOTA | 2104 | CZ | TYR A | | | 18.279 | 42.570 | 46.918 | 1.00 69.08 | 6 |
| ATOM | 2105 | OH | TYR A | | | 18.989 | 42.411 | 45.746 | 1.00 69.01 | 8 |
| ATOM | 2106 | С | TYR A | 264 | | 16.665 | 40.888 | 51.451 | 1.00 43.89 | 6 |
| MOTA | 2107 | 0 | TYR A | | | 15.663 | 40.185 | 51.293 | 1.00 44.80 | 8 |
| ATOM | 2108 | N | LEU A | 265 | | 17.897 | 40.400 | 51.333 | 1.00 40.37 | 7 |
| ATOM | 2109 | CA | LEU A | | | 18.051 | 38.984 | 51.016 | 1.00 38.06 | 6 |
| ATOM . | 2110 | CB | LEU A | 265 | | 19.474 | 38.646 | 50.538 | 1.00 33.48 | 6 |
| ATCM | 2111 | CG | LEU A | | | 19.905 | 39.211 | 49.172 | 1.00 32.43 | 6 |
| ATCM | 2112 | CD1 | LEU A | 265 | | 21.176 | 38.535 | 48.703 | 1.00 26.97 | 6 |

| ATOM | 2113 | CD2 LEU | J A 265 | 18.828 | 38.954 | 48.141 | 1.00 34.41 | 6 |
|--------------|------|-----------------|---------|--------|--------|----------|--------------------------|-----|
| ATOM | 2114 | | J A 265 | 17.665 | | | | |
| ATOM | 2115 | O LEU | J A 265 | 18.125 | | | | 6 |
| ATOM | 2116 | | A 266 | 16.804 | | | | 8 |
| ATOM | 2117 | | A 266 | | | | 1.00 36.21 | 7 |
| | | | | 16.294 | | | 1.00 36.46 | 6 |
| ATOM . | | | A 266 | 17.263 | | | 1.00 37.22 | 6 |
| ATOM | 2119 | | A 266 | 17.190 | | | 1.00 37.41 | 8 |
| MOTA | 2120 | | A 266. | 14.997 | - | 54.653 | 1.00 35.55 | 6 |
| ATOM | 2121 | | A 266 | 14.889 | | 54.568 | 1.00 37.09 | 8 |
| MOTA | 2122 | | A 267 | 14.018 | 37.928 | 55.093 | 1.00 34.33 | 7 |
| ATOM | 2123 | CA LYS | A 267 | 12.750 | 38.493 | 55.532 | 1.00 36.13 | 6 |
| ATOM | 2124 | CB LYS | A. 267 | 11.596 | 37.548 | 55.183 | 1.00 36.11 | 6 |
| MOTA | 2125 | CG LYS | A 267 | 11.503 | 37.222 | 53.705 | | 6 |
| ATOM | 2126 | CD LYS | A 267 | 11.453 | | | 1.00 38.55 | - 6 |
| MOTA | 2127 | CE LYS | A 267 | 11.369 | | | 1.00 41.60 | 6 |
| ATOM | 2128 | | A 267 | 11.503 | | 50.569 | 1.00 42.07 | 7. |
| MOTA | 2129 | | A 267 | 12.791 | | 57.043 | 1.00 34.90 | |
| ATOM | 2130 | | A 267 | 11.758 | | 57.694 | 1.00 34.30 | 6 |
| ATOM | 2131 | | A 268 | 13.998 | | | | 8 |
| ATOM | 2132 | | A 268 | 14.192 | | 57.595 | 1.00 32.82 | 7 |
| ATOM | 2133 | | A 268 | 15.477 | 39.021 | 59.016 | 1.00 31.50 | 6 |
| ATOM | 2134 | | A 268 | | 38.337 | 59.495 | 1.00 34.05 | 6 |
| ATOM | 2135 | CD1 PHE | | 15.379 | 36.839 | 59.604 | 1.00 34.54 | 6. |
| | 2136 | CD1 PHE | | 16.506 | 36.087 | 59.940 | 1.00 35.04 | 6 |
| ATOM | 2137 | | | 14.161 | 36.178 | 59.429 | 1.00 34.57 | 6 |
| MOTA | | CE1 PHE | | 16.423 | 34.691 | 60.108 | 1.00 35.44 | 6 |
| ATOM | 2138 | | A 268 | 14.066 | 34.784 | 59.594 | 1.00 36.00 | 6 |
| ATOM | 2139 | | A 268 | 15.201 | 34.040 | 59.936 | 1.00 34.68 | 6 |
| ATOM | 2140 | | A 268 | 14.319 | 40.530 | 59.190 | 1.00 30.94 | 6 |
| ATOM | 2141 | | A 268 | 14.983 | 41.192 | 58.394 | 1.00 30.27 | 8 |
| ATOM | 2142 | | A 269 | 13.693 | 41.081 | 60.222 | 1.00 32.53 | 7 |
| ATOM | 2143 | | A 269 | 13.760 | 42.527 | 60.448 | 1.00 35.83 | 6 |
| MOTA | 2144 | | A 269 | 12.344 | 43.115 | 60.570 | 1.00 37.23 | 6 |
| MOTA | 2145 | | A 269 | 11.478 | 42.809 | . 59.360 | 1.00 40.75 | 6 |
| ATOM | 2146 | OD1 ASN | | 11.830 | 43.148 | 58.227 | 1.00 43.88 | 8 |
| MOTA | 2147 | ND2 ASN | A 269 | 10.335 | 42.165 | 59.594 | 1.00 39.61 | 7 |
| ATOM | 2148 | C ASN | A 269 | 14.553 | 42.854 | 61.710 | 1.00 35.45 | 6 |
| MOTA | 2149 | O ASN | A 269 | 14.095 | 43.621 | 62.560 | 1.00 41.47 | 8 |
| ATOM | 2150 | N LEU | A 270 | 15.747 | 42.285 | 61.827 | 1.00 33.27 | 7 |
| MOTA | 2151 | CA LEU . | A 270 | 16.571 | 42.510 | 63.004 | 1.00 30.68 | 6 |
| MOTA | 2152 | | A 270 | 17.638 | 41.431 | 63.114 | 1.00 27.41 | 6 |
| MOTA | 2153 | CG LEU | A 270 | 17.140 | 40.002 | 62.988 | 1.00 23.76 | 6 |
| MOTA | 2154 | CD1 LEU | A 270 | 18.222 | 39.106 | 63.543 | 1.00 27.14 | 6 |
| ATOM | 2155 | CD2 LEU 2 | A 270 | 15.855 | 39.801 | 63.772 | 1.00 28.00 | 6 |
| MOTA | 2156 | C LEU | A 270 | 17.258 | 43.856 | 63.033 | 1.00 32.30 | 6 |
| ATOM | 2157 | O LEU | A 270 | 17.347 | 44.554 | 62.017 | 1.00 36.27 | 8 |
| ATOM | 2158 | N SER | A 271 | 17.749 | 44.207 | 64.216 | 1.00 30.33 | 7 |
| MOTA | 2159 | CA SER A | A 271 | 18.465 | 45.457 | 64.424 | 1.00 30.79 | 6 |
| ATOM | 2160 | CB SER A | A 271 | 17.816 | 46.249 | 65.562 | 1.00 29.53 | 6 |
| MOTA | 2161 | OG SER A | | 17.712 | 45.471 | 66.739 | 1.00 30.43 | 8 |
| ATOM | 2162 | C SER A | | 19.911 | 45.109 | 64.768 | 1.00 33:09 | 6 |
| ATOM | 2163 | O SER A | | 20.194 | 43.972 | 65.172 | 1.00 29.64 | 8 |
| ATOM | 2164 | N ASN A | | 20.821 | | 64.586 | 1.00 32.36 | . 7 |
| MOTA | 2165 | CA ASN A | | 22.234 | 45.846 | 64.896 | | |
| ATOM | 2166 | CB ASN A | | 23.036 | | 64.771 | 1.00 31.65 1.00 33.76 | 6 |
| ATOM | 2167 | CG ASN A | | 23.101 | 47.141 | | | 6 |
| MOTA | 2168 | OD1 ASN A | | 23.719 | 47.658 | 63.361 | 1.00 37.76 | 6 |
| ATOM | 2169 | ND2 ASN A | | 22.460 | 48.686 | 63.100 | 1.00 36.12 | 8 |
| | 2170 | | | | 46.952 | 62.437 | 1.00 44.79 | 7 |
| ATOM | 2170 | C ASN A O ASN A | | 22.369 | 45.333 | 66.321 | 1.00 32.61 | 6 |
| MOTA | | | | 22.970 | 44.283 | 66.565 | 1.00 27.95 | 8 |
| MOTA | | N VAL A | | 21.803 | 46.091 | 67.257 | 1.00 33.22 | 7 |
| MOTA | | CA VAL A | | 21.839 | 45.741 | 68.668 | 1.00 35.52 | 6 |
| ATOM | | CB VAL A | | 20.928 | 46.660 | 69.481 | 1.00 37.80 | 6 |
| ATCM | | CG1 VAL A | | 20.987 | 46.276 | 70.964 | 1.00 39.00 | 6 |
| | | CG2 VAL A | | 21.356 | 48.112 | 69.275 | 1.00 38.88 | 6 |
| ATOM | | C VAL A | | 21.416 | 44.300 | 68.908 | 1.00 34.26 | 6 |
| ATOM | 2178 | O VAL A | 273 | 22.060 | 43.580 | 69.679 | 1.00 35.96 | 8 |
| . . . | | • | • • | | | • | • | |

| ATCM | 2179 | N | ALA A 27 | 20.328 | 43.889 | 68.262 | 1.00 32.36 | 7 |
|--------------|--------------|--------|------------------------|------------------|------------------|------------------|--------------------------|--------|
| ATCM | 2180 | CA | ALA A 27 | | | 68.385 | 1.00 31.09 | 6 |
| ATCM | 2181 | CB | ALA A 27 | 18.574 | 42.356 | 67.578 | 1.00 28.88 | 6 |
| ATCM | 2182 | С | ALA A 27 | | 41.588 | 67.861 | 1.00 31.74 | 6 |
| ATCM | 2183 | 0 | ALA A 27 | 21.323 | 40.634 | 68.533 | 1.00 31.54 | 8 |
| ATCM | 2184 | N | PHE A 27 | | 41.879 | 66.655 | 1.00 30.05 | 7 |
| ATOM | 2185 | CA | PHE A 27 | 22.467 | 41.102 | 66.036 | 1.00 31.30 | 6 |
| MOTA | 2186 | CB | PHE A 27 | 22.932 | 41.810 | 64.751 | 1.00 31.54 | 6 |
| MOTA | 2187 | CG | PHE A 27 | | 41.029 | 63.941 | 1.00 31.76 | 6 |
| ATCM | 2188 | CD: | 1 PHE A 27 | | 39.809 | 63.365 | 1.00 32.40 | 6 |
| ATOM | 2189 | CD | 2 PHE A 275 | | 41.529 | 63.729 | 1.00 34:04 | 6 |
| MOTA | 2190 | CE: | 1 PHE A 27 | 24.513 | 39.100 | 62.586 | 1.00 32.27 | 6 |
| MCTA | 2191 | CE | 2 PHE A 27! | | 40.828 | 62.950 | 1.00 33.90 | 6 |
| ATOM | 2192 | CZ | PHE A 27 | 25.793 | 39.613 | 62.378 | 1.00 34.50 | 6 |
| MOTA | 2193 | С | PHE A 27 | | 40.999 | 67.040 | 1.00 29.98 | 6 |
| ATOM | 2194 | 0 | PHE A 275 | | 39.950 | 67.200 | 1.00 29.41 | 8 |
| ATOM | 2195 | N | LEU A 270 | | 42.099 | 67.726 | 1.00 31.22 | 7 |
| ATCM | 2196 | CA | LEU A 276 | | 42.144 | 68.698 | 1.00 32.29 | 6 |
| ATOM | 2197 | CB | LEU A 276 | | 43.594 | 69.141 | 1.00 33.44 | 6 |
| ATCM | 2198 | CG | LEU A 276 | | 43.908 | 70.050 | 1.00 36.01 | 6 |
| ATCM | 2199 | | L LEU A 276 | | 45.391 | 70.025 | 1.00 35.02 | 6 |
| MOTA | 2200 | | 2 LEU A 276 | | 43.433 | 71.467 | 1.00 39.09 | 6 |
| ATOM | 2201 | С | LEU A 276 | | 41.244 | 69.894 | 1.00 32.79 | 6 |
| ATOM | 2202 | 0 | LEU A 276 | | 40.530 | 70.371 | 1.00 30.74 | 8 |
| MOTA | 2203 | N | LYS A 277 | | 41.273 | 70.384 | 1.00 33.95 | 7 |
| ATOM | 2204 | CA | LYS A 277 | | 40.413 | 71.505 | 1.00 36.56 | 6 |
| MOTA | 2205 | CB | LYS A 277 | | 40.588 | 71.902 | 1.00 35.76 | 6 |
| ATOM | 2206 2207 | CD | LYS A 277 | | 41.842 | 72.687 | 1.00 42.31 | 6. |
| ATOM | 2207 | CE | LYS A 277 | | 41.508 40.601 | 74.049 74.865 | 1.00 45.72 | 6 6 |
| ATOM ATOM | 2209 | NZ | LYS A 277 | | 40.378 | 76.244 | 1.00 44.36 | 7 |
| MOTA | 2210 | C | LYS A 277 | | 38.974 | 71.092 | 1.00 37.98 | 6 |
| ATOM | 2211 | ō | LYS A 277 | | 38.179 | 71.845 | 1.00 37.54 | 8 |
| ATOM | 2212 | N | ALA A 278 | | 38.654 | 69.886 | 1.00 37.17 | 7 |
| ATOM | 2213 | CA | ALA A 278 | | 37.311 | 69.323 | 1.00 34.51 | 6 |
| ATOM | 2214 | CB | ALA A 278 | | 37.341 | 67.820 | 1.00 35.38 | 6 |
| ATOM | 2215 | С | ALA A 278 | 24.368 | 36.831 | 69.550 | 1.00 30.63 | 6 |
| ATOM | 2216 | 0 | ALA A 278 | 24.605 | 35.790 | 70.167 | 1.00 27.62 | 8 |
| ATOM | 2217 | N | PHE A 279 | 25.303 | 37.624 | 69.049 | 1.00 29.24 | 7 |
| ATCM | 2218 | CA | PHE A 279 | | 37.347 | 69.167 | 1.00 31.48 | 6 |
| ATOM | 2219 | CB | PHE A 279 | 27.490 | 38.558 | 68.645 | 1.00 33.25 | 6 |
| ATOM | 2220 | CG | PHE A 279 | 28.974 | 38.396 | 68.663 | 1.00 39.28 | 6 |
| ATOM | 2221 | | PHE A 279 | 29.578 | 37.337 | 68.000 | 1.00 41.15 | 6 |
| MOTA | 2222 | | PHE A 279 | 29.776 | 39.328 | 69.315 | 1.00 40.66 | 6 |
| ATCM | 2223 | CE1 | | 30.960 | 37.209 | 67.987 | 1.00 44.22 | 6 |
| ATOM | 2224 | CE2 | | 31.153 | 39.213 | 69.378 | 1.00 41.38 | 6 |
| ATOM | 2225 | CZ | PHE A 279 | 31.750 | 38.152 | 68.614 | 1.00 44.52 | 6 6 |
| ATOM | 2226 | С 0 | PHE A 279 | 27.116 | 37.043 | 70.611 | 1.00 31.81 1.00 27.51 | 8 |
| ATOM | 2227 2228 | N | PHE A 279 ASN A 280 | 27.627 | 35.953 | 70.935 71.503 | 1.00 27.31 | 7 |
| ATOM | 2229 | CA | ASN A 280 | 26.860 | 38.005 37.851 | 72.907 | 1.00 29.26 | 6 |
| MOTA MCTA | 2230 | CB | ASN A 280 | 27.192 26.927 | 39.153 | 73.660 | 1.00 30.39 | 6 |
| ATOM | 2231 | CG | ASN A 280 | 27.907 | 40.245 | 73.278 | 1.00 30.68 | 6 |
| ATOM | 2232 | | ASN A 280 | 29.117 | 40.030 | 73.303 | 1.00 33.34 | 8 |
| ATOM | 2233 | | ASN A 280 | 27.395 | 41.419 | 72.931 | 1.00 27.00 | 7 |
| ATOM | 2234 | C | ASN A 280 | 26.524 | 36.680 | 73.616 | 1.00 30.01 | 6 |
| ATOM | 2235 | õ | ASN A 280 | 27.167 | 36.004 | 74.419 | 1.00 29.58 | 8 |
| ATCM | 2236 | N | ILE A 281 | 25.252 | 36.423 | 73.335 | 1.00 30.46 | 7 |
| MCTA | 2237 | CA | ILE A 281 | 24.594 | 35.291 | 73.983 | 1.00 33.71 | 6 |
| ATOM | 2238 | CB | ILE A 281 | 23.107 | 35.161 | 73.569 | 1.00 36.14 | 6 |
| ATOM | 2239 | CG2 | ILE A 281 | 22.541 | 33.820 | 74.032 | 1.00 36.18 | 6 |
| ATCM | 2240 | CG1 | ILE A 281 | 22.298 | 36.307 | 74.177 | 1.00 33.52 | 6 |
| ATCM | 2241 | CD1 | | 20.835 | 36.243 | 73.834 | 1.00 37.16 | 6 |
| ATOM | 2242 | c | ILE A 281 | 25.330 | 34.006 | 73.631 | 1.00 34.06 | 6 |
| ATOM | 2243 | 0 | ILE A 281 | 25.385 | 33.071 | 74.437 | 1.00 31.94 | 8 |
| ATOM | 2244 | N | VAL A 282 | 25.896 | 33.960 | 72.427 | 1.00 35.31 | 7 |
| | | | | | | | | |

| | | • | |
|-------------|---|----------------------|----------------------|
| ATO | OM 2245 CA .VAL A 282 | 26.654 32.785 72 | |
| ATO | | | .005 1.00 36.45 |
| ATC | | | 524 1.00 35.62 |
| 'ATC | OM 2248 CG2 VAL A 282 | 27.829 31.604 70. | 126 1.00 31.20 |
| | | 25.880 33.080 69. | 646 1.00 34.51 |
| ATC | 202 | 37 040 | 857 1.00 37.80 |
| ATC | VI 11 202 | 20 100 | |
| ATC | M 2251 N ARG A 283 | 30 503 35 | |
| ATO | M 2252 CA ARG A 283 | | 821 1.00 38.45 |
| ATO | | 30 000 | 587 1.00 40.06 |
| ATO | 100 | 30.551 35.272 73. | |
| ATO | | 30.974 35.625 72. | 027 1.00 41.90 |
| ATO | 1210 11 205 | 31.492 37.048 71. | 968 1.00 41.36 |
| | 12.2 12 200 | 32.647 37.206 72. | 040 + 44 - |
| ATO | 203 | 33.162 38.373 73. | 315 1 00 10 5 |
| ATO | | 32.628 39.516 72. | |
| ATO: | | 34 333 | 014 |
| ATO | M 2260 C ARG A 283 | | |
| ATO | M 2261 O ARG A 283 | | |
| ATO | | 30.350 32.862 75. | |
| ATO | | 28.506 34.141 75. | 520 1.00 40 30 7 |
| ATO | | 28.084 33.923 76. | 394 1.00 43.19 6 |
| | | 26.753 34.647 77.1 | 1 C C - 1 0 0 0 0 == |
| ATO | | 26.875 36.176 77.0 | 100 1 00 00 |
| ATO | 020 11 204 | 25.542 36.923 77.1 | |
| IOTA | | | |
| ATO1 | 1 2268 OE2 GLU A 284 | 05 | |
| ATOM | 1 2269 C GLU A 284 | | |
| ATOM | 1 2270 O GLU A 284 | | |
| ATOM | 2271 N VAL A 285 | 0= | |
| ATOM | | 27.186 31.721 76.3 | 54 1.00 34.82 7 |
| ATOM | 205 | 26.975 30.288 76.5 | 51 1.00 30.84 6 |
| ATOM | | 25.842 29.752 75.6 | 47 1.00 27.74 6 |
| | | 25.698 28.253 75.8 | 74 |
| MOTA | | 24.545 30.433 75.9 | 00 |
| ATOM | *************************************** | 28.181 29.366 76.3 | 44 |
| ATOM | | 28.492 28.556 77.2 | 4.4 |
| ATOM | 2278 N PHE A 286 | | |
| MOTA | 2279 CA PHE A 286 | | |
| MOTA | 2280 CB PHE A 286 | 20 000 | |
| MOTA | 2281 CG PHE A 286 | | |
| ATOM | 2282 CD1 PHE A 286 | 28.607 27.095 73.3 | |
| ATOM | 2283 CD2 PHE A 286 | 27.409 27.639 72.8 | 85 1.00 23.90 6 |
| ATOM | 2284 CE1 PHE A 286 | 28.664 25.718 73.60 | |
| ATOM | 2285 CE2 PHE A 286 | 26.281 26.814 72.68 | 81 1.00 24.90 6 |
| | | 27.547 24.892 73.43 | 11 1.00 18.06 6 |
| ATOM | 2286 CZ PHE A 286 | 26.357 25.437 72.94 | |
| ATOM | 2287 C PHE A 286 | 31.368 29.200 74.99 | |
| ATOM | 2288 O PHE A 286 | 32.338 28.566 74.56 | |
| ATOM | 2289 N GLY A 287 | 31.480 30.416 75.52 | |
| ATOM | 229 CA GLY A 287 | 20 500 | , |
| atom | 2291 C GLY A 287 | 22 222 | |
| ATOM | 2292 O GLY A 287 | 20 644 | |
| MOTA | 2293 N. GLU A 288 | | |
| ATOM | 2294 CA GLU A 288 | 34.637 31.849 74.23 | 8 1.00 27.17 7 |
| ATOM | 3295 CB GLU A 288 | 35.274 32.291 72.99 | 6 1.00 33.20 6 |
| ATOM | | 36.680 32.828 73.26 | |
| | | 36.726 34.104 74.08 | 3 1.00 41.67 6 |
| ATOM | 2297 CD GLU A 288 | 35.970 35.231 73.42 | |
| ATOM | 2298 OE1 GLU A 288 | 36.221 35.493 72.22 | |
| MOTA | 2299 OE2 GLU A 288 | 25 45- | |
| ATOM | 2300 C GLU A 288 | 25 222 | |
| MOTA | 2301 O GLU A 288 | | |
| ATOM | 2302 N GLY A 289 | 25 250 - | _ |
| ATOM | 2303 CA GLY A 289 | 35.268 31.619 70.66 | |
| ATOM | 2224 | 35.373 30.698 69.549 | 5 1.00 29.58 6 |
| ATOM | - 001 // 205 | 35.948 31.372 68.307 | 7 1.00 27.42 5 |
| | | 36.556 32.437 68.398 | |
| ATOM | 2306 N VAL A 290 | 35.764 30.758 67.143 | |
| ATOM | 2307 CA VAL A 290 | 36.277 31.349 65.907 | |
| ATOM | 2308 CB VAL A 290 | 37.014 30.301 65.037 | |
| MOTA | 2309 CG1 VAL A 290 | 37.616 30.976 63.813 | 1.00 25.25 6 |
| MOTA | 2310 CG2 VAL A 290 | | |
| | | 38.100 29.632 65.852 | 1.00 17.33 6 |
| | | • | |

| | | | | | | | | | | _ |
|-------|------|-----|-------|-------|--------|----|--------|---------|------------|-----|
| . mov | 2311 | С | VAL A | 290 | 35.13 | 7 | 31.975 | 65.105 | 1.00 25.97 | 6 |
| MOTA | | ō | VAL A | | 34.21 | 8 | 31.279 | 64.672 | 1.00 22.32 | 8 |
| MOTA | 2312 | | TYR A | | 35.21 | | 33.293 | 64.914 | 1.00 27.33 | 7 |
| MOTA | 2313 | N | | | | | 34.052 | 64.203 | 1.00 26.69 | 6 |
| ATOM | 2314 | CA | TYR A | | 34.18 | | | 64.939 | 1.00 25.51 | 6 |
| ATOM | 2315 | CB | TYR A | | 33.92 | | 35.356 | | 1.00 28.73 | 6 |
| ATOM | 2316 | CG | TYR A | 291 | 33.93 | 5 | 35.178 | 66.435 | | |
| | 2317 | CD1 | TYR A | 291 | 35.02 | 5 | 35.596 | 67.191 | 1.00 29.72 | 6 |
| MOTA | | CEI | TYR A | 291 | 35.05 | 9 | 35.414 | 68.563 | 1.00 29.53 | 6 |
| ATOM | 2318 | CDI | TYR A | 201 | 32.87 | | 34.565 | 67.094 | 1.00 27.39 | 6 |
| MOTA | 2319 | | | | | | 34.377 | 68.466 | 1.00 31.03 | 6 |
| ATOM | 2320 | CE2 | TYR A | | 32.89 | | | 69.194 | 1.00 31.85 | 6 |
| ATOM | 2321 | CZ | TYR A | | 33.99 | | 34.808 | 70 563 | 1.00 38.03 | 8 . |
| ATOM | 2322 | OH | TYR A | 291 | 34.03 | | 34.647 | 70.562 | | 6 |
| | 2323 | С | TYR A | 291 | 34.52 | 7 | 34.345 | 62.745 | 1.00 27.99 | |
| ATOM | 2324 | . 0 | TYR A | | 35.60 | 8 | 34.843 | 62.415 | 1.00 24.83 | 8 |
| ATOM | | N | LEU A | | 33.56 | | 34.042 | 61.880 | 1.00 30.17 | 7 |
| MOTA | 2325 | | LEU A | | 33.72 | | 34.220 | 60.441 | 1.00 28.26 | 6 |
| MOTA | 2326 | CA | | | | | 32.861 | 59.741 | 1.00 27.70 | 6 |
| ATOM | 2327 | CB | LEU A | | 33.56 | | | 60.435 | 1.00 24.64 | 6 |
| MOTA | 2328 | CG | LEU A | 292 | 34.19 | | 31.643 | | 1.00 24.66 | 6 |
| ATOM | 2329 | CD1 | LEU A | 292 | 33.86 | 7 | 30.380 | 59.661 | 1.00 24.00 | 6 |
| | 2330 | CD2 | LEU A | 292 | 35.68 | 16 | 31.825 | 60.553 | 1.00 23.19 | |
| MOTA | 2331 | C | LEU A | 292 | 32.64 | 9 | 35.175 | 59.944 | 1.00 25.59 | 6 |
| ATOM | | | LEU A | 292 | 31.64 | | 35.394 | 60.611 | 1.00 18.11 | 8 |
| MOTA | 2332 | 0 | GLY A | 293 | 32.86 | | 35.749 | 58.770 | 1.00 28.55 | 7 |
| MOTA | 2333 | N | GLI A | 222 | 31.87 | | 36.653 | 58.223 | 1.00 31.26 | 6 |
| ATOM | 2334 | CA | GLY A | | | | 35.815 | 57.714 | 1.00 34.84 | 6 |
| ATOM' | 2335 | С | GLY A | | 30.72 | | | 58.234 | 1.00 34.11 | 8 |
| ATOM | 2336 | 0 | GLY A | 293 | 30.46 | | 34.724 | | 1.00 35.34 | 7 |
| ATOM | 2337 | N | GLY A | 294 | 30.03 | | 36.312 | 56.689 | | 6 |
| | 2338 | CA | GLY A | 294 . | 28.91 | 8 | 35.581 | 56.124 | 1.00 34.84 | |
| MOTA | 2339 | C | GLY A | | 28.14 | 12 | 36.445 | 55.155 | 1.00 34.79 | 6 |
| MOTA | | | GLY A | | 28.64 | | 37.473 | 54.699 | 1.00 37.05 | 8 |
| MOTA | 2340 | 0 | GLY A | 205 | 26.91 | | 36.035 | 54.842 | 1.00 31.87 | 7 |
| MOTA | 2341 | N | | | | | 36.806 | 53.925 | 1.00 27.78 | 6 |
| MOTA | 2342 | CA | GLY A | | 26.10 | | | 54.378 | 1.00 27.09 | 6 |
| MOTA | 2343 | С | GLY A | | 25.96 | | 38.245 | | 1.00 27.03 | 8 |
| ATOM | 2344 | .0 | GLY A | 295 | 26.19 | | 38.558 | 55.546 | | 7 |
| | 2345 | N | GLY A | 296 | 25.59 | 96 | 39.119 | 53.450 | 1.00 24.67 | 6 |
| MOTA | 2346 | CA | GLY A | 296 | 25.44 | 40 | 40.527 | 53.757 | 1.00 25.28 | |
| MOTA | | c. | GLY A | | 25.56 | 52 | 41.262 | 52.446 | 1.00 27.64 | 6 |
| ATOM | 2347 | | GLY A | 296 | 26.59 | | 41.163 | 51.771 | 1.00 26.65 | 8 |
| MOTA | 2348 | 0 | | | 24.52 | | 42.009 | 52.078 | 1.00 30.21 | 7 |
| ATOM | 2349 | N | TYR A | | 24.54 | | 42.704 | 50.801 | 1.00 30.62 | 6 |
| MOTA | 2350 | CA | TYR A | | | | 42.011 | 49.859 | 1.00 29.50 | 6 |
| ATOM | 2351 | CB | TYR A | | 23.56 | | | 49.953 | 1.00 30.33 | 6 |
| ATOM | 2352 | CG | TYR A | 297 | 23.73 | | 40.516 | | 1.00 30.86 | 6 |
| MOTA | 2353 | CD1 | TYR A | 297 | 23.1 | | 39.810 | 51.031 | 1.00 30.74 | 6 |
| | 2354 | CE1 | TYR A | 297 | 23.4 | 50 | 38.449 | 51.226 | 1.00 30.74 | 6 |
| MOTA | 2355 | CD2 | TYR A | 297 | 24.5 | 38 | 39.824 | 49.062 | 1.00 31.20 | |
| ATOM | | CE2 | | 297 | 24.8 | | 38.460 | 49.247 | 1.00 32 08 | 6 |
| MOTA | 2356 | | TYR A | 207 | 24.2 | | 37.781 | 50.332 | 1.00 30.92 | 6 |
| MOTA | 2357 | CZ | TIKA | 207 | . 24.5 | | 36.440 | 50.509 | 1.00 29 60 | 8 |
| MOTA | 2358 | OH | TYR A | | | | | 50.875 | 1.00 32.07 | 6 |
| ATOM | 2359 | С | TYR A | | 24.2 | | 44.195 | 49.840 | 1.00 33.83 | 8 |
| ATOM | 2360 | 0 | TYR A | 297 | 24.1 | | 44.849 | | 1.00 31.41 | 7 |
| | 2361 | N | HIS A | 298 | 24.1 | | | 52.094 | 1.00 31.47 | 6 |
| ATOM | 2362 | CA | HIS A | 298 | 23.9 | 61 | 46.153 | 52.289 | 1.00 33.94 | |
| MOTA | | CB | HIS A | 298 | 22.7 | | 46.430 | 53.194 | 1.00 34.75 | 6 |
| ATOM | 2363 | | HIS A | 208 | 22.3 | | 47.880 | 53.256 | 1.00 35.16 | 6 |
| MOTA | 2364 | CG | DID A | 200 | 22.5 | | 48.809 | 54.224 | 1.00 35.72 | 6 |
| ATOM | 2365 | CD2 | HIS A | 290 | | | | 52.205 | 1.00 34.10 | 7 |
| ATOM | 2366 | ND1 | HIS A | 298 | 21.7 | | 48.538 | 52.522 | 1.00 31.84 | 6 |
| ATOM | 2367 | CE1 | HIS A | 298 | 21.6 | | 49.809 | | 1.00 35.46 | 7 |
| ATOM | 2368 | NE2 | HIS A | 298 | 22.0 | | 50.000 | 53.742 | 1.00 36.21 | 6 |
| | 2369 | С | HIS A | 298 | 25.2 | 13 | 46.697 | 52.962 | 1.00 30.41 | |
| ATOM | _ | ō | HIS A | 298 | 25.4 | | 46.405 | 54.133 | 1.00 33.83 | 8 |
| ATOM | 2370 | | PRO A | 299 | 25.9 | | 47.519 | 52.234 | 1.00 36.69 | 7 |
| ATOM | 2371 | N | | | 25.6 | | 47.997 | 50.881 | 1.00 35.57 | 6 |
| MOTA | 2372 | CD | PRO A | 200 | | | 48.142 | 52,689 | | 6 |
| ATOM | 2373 | CA | PRO A | 299 | 27.2 | | | 51.525 | | 6 |
| ATOM | 2374 | CB | PRO A | 299 | 27.5 | | 49.073 | | | 6 |
| ATOM | 2375 | CG | PRO A | 299 | 26.2 | | 49.399 | C 4 000 | | 6 |
| | 2376 | c | PRO A | 299 | 27.0 | 45 | 48.886 | 54.000 | 1.00 34.47 | J |
| MOTA | 0/دن | _ | | • | | | | - | | |
| | | | | • | | | • | | | |
| | | | | | | | | | | |

| ATOM | 1 2377 O PRO A 299 | 27. | 781 10 c | 70 54 06 | | |
|--------------|--|------------------|------------------|-----------|------------|--------|
| MOTA | | 26. | | | 25.0 | |
| ATOM | | 25. | | | | |
| ATOM | | | | | | |
| ATOM | | 24. | - · · · · - · · | | | |
| ATOM | | 24.0 | | | | 6 |
| ATOM | | 25.3 | | | | 6 |
| ATOM | | 25.4 | | 05 51.907 | | 6 |
| | | 24.0 | 016 53.79 | | 1.00 35.92 | 6 |
| MOTA | | 24.0 | | 93 53.334 | 1.00 36.78 | 6 |
| ATOM | | 24.8 | | | 1.00 38.09 | 6 |
| ATOM | | 24.9 | | 4 51.251 | 1.00 37.68 | 8 |
| MOTA | | 25.4 | 97 49.54 | 6 56.3.69 | 1.00 31.10 | 6 |
| ATOM | | 26.0 | 62 49.69 | 2 57.440 | 1.00 30.62 | |
| ATOM | | 24.6 | 61 48.54 | | | |
| ATOM | | 24.3 | 23 47.54 | | | |
| ATOM | | 23.2 | 16 46.60 | | | 6 |
| ATOM | | 25.5 | 39 46.72 | | | |
| ATOM | | 25.8 | | | 1.00 31.91 | 8 |
| MOTA | | 26.2 | | | | |
| ATOM | 2396 CA LEU A 302 | 27.4 | | | 1.00 30.55 | 7 6 |
| ATOM | 2397 CB LEU A 302 | 28.0 | | | 1.00 31.83 | |
| ATOM | 2398 CG LEU A 302 | . 29.3 | | | 1.00 30.01 | 6 |
| ATOM | 2399 CD1 LEU A 302 | 29.4 | | | 1.00 32.09 | 6 |
| ATOM | 2400 CD2 LEU A 302 | 30.4 | 75 45.07 | 7 55.762 | 1.00 32.03 | 6 |
| ATOM | 2401 C LEU A 302 | 28.4 | 18 46.13 | | 1.00 32.23 | 6 |
| ATOM | 2402 O LEU A 302 | 28.79 | | 58.746 | 1.00 27.68 | 6 |
| MOTA | 2403 N ALA A 303 | 28.84 | | | 1.00 27.88 | 8 |
| ATOM | 2404 CA ALA A 303 | 29.83 | | | 1.00 27.92 | 7 |
| ATOM | 2405 CB ALA A 303 | 30.02 | | | 1.00 23.62 | 6 |
| MOTA | 2406 C ALA A 303 | 29.39 | | 59.305 | 1.00 25.06 | 6 6 |
| ATOM | 2407 O ALA A 303 | 30.08 | | | 1.00 26.90 | 8 |
| ATOM | 2408 N ARG A 304 | 28.25 | | | 1.00 24.06 | 7 |
| ATOM | 2409 CA ARG A 304 | 27.79 | 4 49.382 | | 1.00 24.37 | 6 |
| MOTA | 2410 CB ARG A 304 . | 26.42 | | | 1.00 23.99 | 6 |
| MOTA | 2411 CG ARG A 304 | 26.32 | | | 1.00 28.77 | 6 |
| ATOM | 2412 CD ARG A 304 | 25.10 | | | 1.00 29.96 | 6 |
| ATOM | 2413 NE ARG A 304 | 23.94 | | 60.369 | 1.00 36.43 | 7 |
| ATOM | 2414 CZ ARG A 304 | 22.89 | | 61.110 | 1.00 37.01 | 6 |
| ATOM | 2415 NH1 ARG A 304 | 22.85 | | 61.713 | 1.00 36.37 | 7 |
| MOTA | 2416 NH2 ARG A 304 | 21.89 | | 61.269 | 1.00 34.36 | 7 |
| ATOM | 2417 C ARG A 304 | 27.72 | | 61.691 | 1.00 24.24 | 6 |
| ATOM ATOM | 2418 O ARG A 304 2419 N ALA A 305 | 28.34 | | 62.762 | 1.00 22.34 | 8 |
| ATOM | | 26.99 | | 61.221 | 1.00 24.51 | 7 |
| ATOM | 2420 CA ALA A 305 2421 CB ALA A 305 | 26.80 | | 61.959 | 1.00 22.70 | 6 |
| ATOM | 2422 C ALA : 305 | 25.880 | | 61.175 | 1.00 18.13 | 6 . |
| ATOM | 2422 C ALA . 305 | 28.089 | | 62.351 | 1.00 23.33 | · 6 |
| ATOM | 2424 N TRP 306 | 28.237 | | 63.506 | 1.00 21.51 | 8 |
| ATOM | 2425 CA TRP A 306 | 29.016 | – | 61.411 | 1.00 22.79 | 7 |
| ATOM | 2426 CB TRP A 306 | 30.244 | | 61.764 | 1.00 24.33 | 6 |
| ATOM | 2427 CG TRP A 306 | 31.029 | 43.842 | 60.524 | 1.00 26.93 | 6 |
| ATOM | 2428 CD2 TRP A 306 | 30.604 | 42.503 | 59.952 | 1.00 27.96 | 6 |
| ATOM | 2429 CE2 TRP A 306 | 30.861 | | 58.629 | 1.00 26.38 | 6 |
| MOTA | 2430 CE3 TRP A 306 | 30.366 31.462 | | 58.570 | 1.00 24.96 | 6 . |
| ATOM | 2431 CD1 TRP A 306 | | -0.505 | 57.490 | 1.00 23.00 | 6 |
| MOTA | 2432 NE1 TRP A 306 | 29.983 | | 60.620 | 1.00 28.53 | 6 |
| MOTA | 2433 CZ2 TRP A 306 | 29.837 | | 59.797 | 1.00 25.62 | 7 |
| ATOM | 2434 CZ3 TRP A 306 | 30.450 | | 57.414 | 1.00 24.51 | 6 |
| MOTA | 2435 CH2 TRP A 306 | 31.548 | | 56.343 | 1.00 25.37 | 6 |
| ATOM | 2436 C TRP A 306 | 31.042 | 40.465 | 56.315 | 1.00 24.20 | 6 |
| TOM | 2437 O TRP A 306 | 31.129 | 45.108 | 62.676 | 1.00 26.51 | 6 |
| TOM | 2438 N THR A 307 | 31.908 31.003 | 44.570 | | 1.00 25.07 | 8 |
| TOM | 2439 CA THR A 307 | 31.785 | 46.427 | | 1.00 28.08 | 7 |
| | 2440 CB THR A 307 | 31.484 | 47.323 | | 1.00 27.91 | 6. |
| TOM | 2441 OG1 THR A 307 | 31.994 | 48.796 | 63.100 | 1.00 27.86 | 6 |
| TOH | 2442 CG2 THR A 307 | 32.120 | 49.119 49.704 | 61.799 | 1.00 30.17 | 8 |
| | | 120 | 43.704 | 64.137 | 1.00 24.72 | 6 |
| | | | | | | _ |

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Figure 17-38

| | _ | | | | | | | |
|-------|------|--------|-------------|----------|---------|--------|------------|----|
| ATOM | 2443 | С | THR A 307 | 31.441 | 47.041 | 64.863 | 1.00 29.35 | 6 |
| MOTA | 2444 | o. | THR A 307 | 32.316 | 46.989 | 65.725 | 1.00 32.56 | 8 |
| MOTA | 2445 | N | LEU A 308 | 30.159 | 46.857 | 65.135 | 1.00 30.60 | 7 |
| MOTA | 2446 | CA | LEU A 308 | 29.740 | 46.555 | 66.490 | 1.00 33.69 | 6 |
| ATOM | 2447 | CB | | 28.256 | 46.215 | 66.525 | 1.00 34.48 | 6 |
| MOTA | 2448 | CG | | 27.338 | 47.337 | 66.058 | 1.00 34.79 | 6 |
| MOTA | 2449 | CD | | 25.903 | 46.887 | 66.153 | 1.00 31.98 | |
| | | | - | | | | | 6 |
| ATOM | 2450 | CD | | 27.569 | 48.542 | 66.924 | 1.00 36.96 | 6 |
| MOTA | 2451 | C | LEU A 308 | 30.531 | 45.353 | 66.965 | 1.00 34.57 | 6 |
| ATOM | 2452 | 0 | LEU A 308 | 31.230 | 45.417 | 67.975 | 1.00 33.75 | 8 |
| ATOM | 2453 | N | ILE A 309 | . 30.423 | 44.262 | 66.208 | 1.00 35.78 | 7 |
| ATOM | 2454 | CA | ILE A 309 | 31.108 | 43.017 | 66.540 | 1.00 35.87 | 6 |
| ATOM | 2455 | CB | ILE A 309 | 30.939 | 41.949 | 65.431 | 1.00 34.95 | 6 |
| MOTA | 2456 | CG: | 2 ILE A 309 | 31.733 | 40.695 | 65.799 | 1.00 31.21 | 6 |
| MOTA | 2457 | CG: | 1 ILE A 309 | 29.445 | 41.631 | 65.212 | 1.00 34.25 | 6 |
| ATOM | 2458 | CD | | 28.726 | 41.014 | 66.407 | 1.00 25.04 | 6 |
| ATOM | 2459 | C | ILE A 309 | 32.589 | 43.238 | 66.772 | 1.00 35.81 | 6 |
| ATOM | 2460 | ō | ILE A 309 | 33.183 | 42.617 | 67.657 | 1.00 38.19 | 8 |
| | 2461 | N | TRP A 310 | 33.197 | 44.111 | 65.977 | | 7 |
| ATOM | | | TRP A 310 | | | | 1.00 36.10 | |
| MOTA | 2462 | CA | | 34.612 | 44.384 | 66.169 | 1.00 35.26 | 6 |
| ATOM | 2463 | CB | TRP A 310 | 35.150 | 45.311 | 65.075 | 1.00 32.61 | 6 |
| MOTA | 2464 | CG | TRP A 310 | 36.619 | 45.588 | 65.220 | 1.00 30.79 | 6 |
| ATOM | 2465 | CD | | 37.679 | 44.620 | 65.274 | 1.00 29.93 | 6 |
| MOTA | 2466 | CE | | 38.882 | 45.330 | 65.474 | 1.00 28.42 | 6 |
| ATOM | 2467 | CE: | | 37.731 | 43.224 | 65.174 | 1.00 31.59 | 6 |
| MOTA | 2468 | CD: | 1 TRP A 310 | 37.206 | 46.804 | 65.380 | 1.00 30.62 | 6 |
| ATOM | 2469 | NE: | I TRP A 310 | 38.565 | 46.659 | 65.536 | 1.00 29.37 | 7 |
| ATOM | 2470 | CZ | TRP A 310 | 40.126 | 44.691 | 65.578 | 1.00 27.91 | 6 |
| ATOM | 2471 | CZ3 | 3 TRP A 310 | 38.978 | 42.585 | 65.279 | 1.00 28.06 | 6 |
| ATOM- | 2472 | CH | TRP A 310 | 40.150 | 43.322 | 65.479 | 1.00 26.50 | 6 |
| ATOM | 2473 | C | TRP A 310 | 34.744 | 45.040 | 67.545 | 1.00 36.00 | 6 |
| ATOM | 2474 | ō | TRP A 310 | 35.365 | 44.476 | 68.440 | 1.00 36.24 | 8 |
| ATOM | 2475 | N | CYS A 311 | 34.134 | 46.213 | | 1.00 34.57 | 7 |
| | 2476 | CA | CYS A 311 | 34.183 | 46.937 | 68.985 | 1.00 32.82 | 6 |
| MOTA | | | CYS A 311 | | | | | |
| MOTA | 2477 | CB | | 33.169 | 48.085 | 68.996 | 1.00 35.62 | .6 |
| ATOM | 2478 | SG | CYS A 311 | 33.439 | 49.401 | 67.796 | 1.00 32.36 | 16 |
| MOTA | 2479 | C | CYS A 311 | 33.912 | 46.061 | 70.206 | 1.00 32.01 | 6 |
| MOTA | 2480 | 0 | CYS A 311 | 34.452 | 46.313 | 71.280 | 1.00 29.82 | 8 |
| MOTA | 2481 | N | GLU A 312 | 33.062 | 45.049 | 70.053 | 1.00 32.57 | 7 |
| MOTA | 2482 | CA | GLU A 312 | 32.731 | 44.159 | 71.171 | 1.00 33.86 | 6 |
| ATOM | 2483 | CB | GLU A 312 | 31.557 | 43.252 | 70.807 | 1.00 34.19 | 6 |
| ATCM | 2484 | CG | GLU A 312 | 30.442 | 43.185 | 71.844 | 1.00 40.27 | 6 |
| MOTA | 2485 | CD | GLU A 312 | 30.923 | 42.821 | 73.239 | 1.00 43.80 | 6 |
| MOTA | 2486 | OE1 | GLU A 312 | 31.685 | 41.831 | 73.383 | 1.00 44.81 | 8 |
| ATOM | 2487 | OE2 | GLU A 312 | 30.516 | 43.522 | 74.195 | 1.00 41.54 | 8 |
| ATOM | 2488 | С | GLU A 312 | 33.953 | 43.298 | 71.456 | 1.00 33.77 | 6 |
| ATOM | 2489 | 0 | GLU A 312 | 34.253 | 42.957 | 72.603 | 1.00 32.07 | 8 |
| ATOM | 2490 | N | LEU A 313 | 34.647 | 42.945 | 70.382 | 1.00 33.45 | 7 |
| ATOM | 2491 | CA | LEU A 313 | 35.848 | 42.135 | 70.473 | 1.00 32.89 | 6 |
| | 2492 | CB | LEU A 313 | 36.172 | 41.513 | 69.115 | 1.00 32.14 | 6 |
| MOTA | 2493 | CG | LEU A 313 | 35.154 | 40.493 | 68.626 | 1.00 27.73 | 6 |
| ATOM | | | | | | | 1.00 30.39 | _ |
| ATCM | 2494 | | LEU A 313 | 35.587 | 39.956 | | | 6 |
| ATOM | 2495 | | LEU A 313 | 35.053 | 39.367 | 69.648 | 1.00 27.87 | 6 |
| ATOM | 2496 | С | LEU A 313 | 36.976 | | 70.903 | 1.00 31.64 | 6 |
| ATOM | 2497 | 0 | LEU A 313 | 37.605 | 42.793 | 71.925 | 1.00 31.74 | 8 |
| ATCM | 2498 | N | SER A 314 | 37.206 | 44.064 | 70.099 | 1.00 33.49 | 7 |
| ATOM | 2499 | CA | SER A 314 | 38.232 | 45.067 | 70.328 | 1.00 35.59 | 6 |
| ATOM | 2500 | CB | SER A 314 | 38.107 | 46.154 | 69.256 | 1.00 36.47 | 6 |
| ATOM | 2501 | 0G | SER A 314 | 39.141 | 47.120 | 69.353 | 1.00 44.55 | 8 |
| ATCM | 2502 | c | SER A 314 | 38.046 | 45.661 | 71.730 | 1.30 37.82 | 6 |
| ATOM | 2503 | ŏ | SER A 314 | 39.015 | 46.043 | 72.395 | 1.00 37.32 | 8 |
| | 2504 | N | GLY A 315 | 36.794 | 45.725 | 72.175 | 1.00 38.05 | 7 |
| ATCM | 2505 | CA | GLY A 315 | 36.506 | 46'.243 | 73.498 | 1.00 42.42 | 6 |
| ATCM | 2506 | C | GLY A 315 | 36.295 | 47.744 | 73.568 | 1.00 46.80 | 6 |
| MOTA | | | GLY A 315 | 35.923 | | 74.618 | 1.00 47.85 | 8 |
| ATOM | 2507 | O N | | | 48.276 | | 1.00 48.90 | |
| ATCM | 2508 | N | ARG A 316 | 36.518 | 48.438 | 72.458 | 1.00 40.30 | 7 |

| ATOM | 2509 CA ARG A 316 | 36.346 49.885 72.448 1.00 52.27 6 |
|-------|--------------------|---|
| ATOM | | 72.440 1.00 52.27 |
| ATOM | | 71.203 1.00 33.60 6 |
| ATOM | | 55.507 63.500 1.00 52.11 6 |
| ATOM | 12.0 11 520 | 1.00 33.76 |
| | | 75.015 1.00 33.07 |
| ATOM | | 40.135 50.221 68,383 1.00 55.34 6 |
| MOTA | 2515 NH1 ARG A 316 | 40.110 51 253 67 552 1 00 55 44 7 |
| MOTA | 2516 NH2 ARG A 316 | 41.266 49.546 68.569 1.00 55 80 7 |
| MOTA | 2517 C ARG A 316 | 34 992 50 343 80 301 |
| MOTA | 2518 O ARG A 316 | 34 075 40 701 71 650 |
| MOTA | 2519 N GLU A 317 | 2.00 34.50 6 |
| MOTA | 2520 CA GLU A.317 | 33 105 51 000 |
| MOTA | 2521 CB GLU A 317 | 22 111 52 120 52.07 |
| ATOM | 2522 CG GLU A 317 | |
| ATOM | 2523 CD GLU A 317 | 22 252 54 444 |
| ATOM | 2524 OE1 GLU A 317 | 33.353 51.912 76.361 1.00 64.62 6 |
| ATOM | 2525 OE2 GLU A 317 | 33.025 51.741 77.556 1.00 64.59 8 |
| | 2526 C GLU A 317 | 34.305 51.302 75.832 1.00 68.64 8 |
| MOTA | | 32.642 52.256 71.843 1.00 51 27 6 |
| MOTA | 2527 O GLU A 317 | 33.270 52.983 71.077 1.00 49.34 8 |
| ATOM | 2528 N VAL A 318 | 31.457 51.733 71.548 1.00 51.30 7 |
| MOTA | 2529 CA VAL A 318 | 30.780 51.962 70.280 1.00 48.80 6 |
| ATOM | 2530 CB VAL A 318 | 29.522 51.071 70.169 1.00 47.11 6 |
| MOTA | 2531 CG1 VAL A 318 | 70 075 51 077 60 000 |
| MOTA | 2532 CG2 VAL A 318 | 20 205 40 521 |
| ATOM | 2533 C VAL A 318 | 30 340 53 444 |
| MOTA | 2534 O VAL A 318 | 20 511 52 007 70 000 |
| MOTA | 2535 N PRO A 319 | 20 005 |
| MOTA | 2536 CD PRO A 319 | 7 |
| ATOM | 2537 CA PRO A 319 | 30 530 55 550 |
| ATOM | 2538 CB PRO A 319 | |
| ATOM | 2539 CG PRO A 319 | 7 |
| ATOM | 2540 C PRO A 319 | 31.612 54.802 67.141 1.00 50.17 6 |
| MOTA | 319 | 29.052 55.679 68.764 1.00 55.84 6 |
| | | 28.531 54.913 67.953 1.00 56.06 8 |
| ATOM | | 28.369 56.624 69.402 1.00 59.20 7 |
| MOTA | 2543 CA GLU A 320 | 26.942 56.804 69.167 1.00 62.61 6 |
| ATOM | 2544 CB GLU A 320 | 26.302 57.588 70.313 1.00 65.59 6 |
| ATOM | 2545 CG GLU A 320 | 26.727 59.042 70.365 1.00 73.01 6 |
| ATOM | 2546 CD GLU A 320 | 26.007 59.823 71.451 1.00 76.93 6 |
| ATOM | 2547 OE1 GLU A 320 | 24.755 59.832 71.446 1.00 77.37 8 |
| ATOM | 2548 OE2 GLU A 320 | 26.697 60.431 72.303 1.00 79.46 8 |
| ATOM | 2549 C GLU A 320 | 26.698 57.551 67.863 1.00 61.40 6 |
| ATOM | 2550 O GLU A 320 | 25.663 58.197 67.699 1.00 62.33 8 |
| MOTA | 2551 N LYS A 321 | 27.650 57.463 66.939 1.00 59.47 7 |
| ATOM | 2552 CA LYS A 321 | 27.519 58.150 65.662 1.00 59.54 6 |
| ATOM | 2553 CB LYS A 321 | 27 240 50 540 |
| ATOM | 2554 CG LYS A 321 | 22 (20 50 50 50 50 50 50 50 50 50 50 50 50 50 |
| ATOM | 2555 CD LYS A 321 | 13 160 70 701 |
| ATOM | 2556 CE LYS A 321 | 3) ECA CO OAS CO OAS |
| MOTA | 2557 NZ LYS A 321 | 20 500 |
| ATOM | 2558 C LYS A 321 | 20 766 57 546 54 555 |
| ATOM | 2559 O LYS A 321 | 20 045 |
| ATOM | 2560 N LEU A 322 | 20 500 |
| MOTA | | 28.608 58.146 63.500 1.00 57.55 7 |
| | | 29.702 58.002 62.543 1.00 54.72 6 |
| ATOM | | 29.171 57.450 61.214 1.00 52.96 6 |
| ATOM | 2563 CG LEU A 322 | 28.141 56.316 61.295 1.00 52.97 6 |
| ATCM | 2564 CD1 LEU A 322 | 27.708 55.932 59.899 1.00 49.01 6 |
| MOTA | 2565 CD2 LEU A 322 | 28.716 55.115 62.035 1.00 54.73 6 |
| MOTA | 2566 C LEU A 322 | 30.250 59.406 62.313 1.00 53.47 .6 |
| MOTA | 2567 O LEU A 322 | 29.512 60.383 62.464 1.00 53.39 8 |
| MOTA | 2568 N ASN A 323 | 31.530 59.521 61.965 1.00 51.43 7 |
| MOTA | 2569 CA ASN A 323 | 32.089 60.842 61.706 1.00 50.32 6 |
| MOTA | 2570 CB ASN A 323 | 33.591 60.905 62.035 1.00 52.31 6 |
| MOTA | 2571 CG ASN A 323 | 34.428 59.964 61.189 1.00 55.06 6 |
| TOM | 2572 OD1 ASN A 323 | 24 206 70 |
| ATOM | 2573 ND2 ASN A 323 | 25 405 |
| MOTA | 2574 C ASN A 323 | 21 042 |
| 11011 | 25/4 C ASM A 323 | 31.843 61.199 60.243 1.00 48.63 6 |

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| ATOM | 2575 | 0 | ASN A 32 | 3 31.135 | 60.479 | 59.538 | 1.00 47.52 | 8 |
|--------------|--------------|----------|----------------------|----------|------------------|------------------|--------------------------|--------|
| ATOM | 2576 | N | ASN A 32 | | 62.304 | 59.792 | 1.00 47.66 | 7 |
| ATOM | 2577 | CA | ASN A 32 | | 62.769 | 58.419 | 1.00 49.25 | 6 |
| ATOM | 2578 | CB | ASN A 32 | | 64.200 | 58.292 | 1.00 50.73 | 6 |
| ATOM | 2579 | ÇG | ASN A 32 | | 65.154 | 59.205 | 1.00 53.83 | 6 |
| ATOM | 2580 | | L ASN A 32 | | 65.314 | 59.096 | 1.00 56.90 | 8 |
| ATOM | 2581 | | ASN A 32 | | 65.789 | 60.119 | 1.00 54.93 | 7 |
| ATOM | 2582 | C | ASN A 32 | | 61.891 | 57.367 | 1.00 49.34 | 6 |
| ATOM | 2583 | ŏ | ASN A 32 | | 61.502 | 56.379 | 1.00 47.22 | 8 |
| ATOM | 2584 | N | LYS A 32 | | 61.590 | 57.586 | 1.00 48.27 | 7 |
| ATOM | 2585 | CA | LYS A 32 | | 60.759 | 56.676 | 1.00 46.57 | 6 |
| ATOM | 2586 | CB | LYS A 32 | | 60.453 | 57.305 | 1.00 49.94 | 6 |
| MOTA | 2587 | CG | LYS A 32 | | 59.737 | 56.399 | 1.00 54.75 | 6 |
| ATOM | 2588 | CD | LYS A 32 | | 59.329 | 57.173 | 1.00 58.22 | 6 |
| ATOM | 2589 | CE | LYS A 32 | | 60.521 | 57.844 | 1.00 58.35 | 6 |
| ATOM | 2590 | NZ | LYS A 32 | | 60.128 | 58.566 | 1.00 59.81 | 7 |
| ATOM | 2591 | c | LYS A 32 | | 59.458 | 56.410 | 1.00 44.85 | 6 |
| ATOM | 2592 | ŏ | LYS A 32 | | 59.027 | 55.263 | 1.00 43.59 | |
| ATOM | 2593 | N | ALA A 32 | | 58.843 | 57.483 | 1.00 42.27 | . 7 |
| ATOM | 2594 | CA | ALA A 32 | | 57.597 | 57.387 | 1.00 40.91 | 6 |
| ATOM | 2595 | CB | ALA A 32 | | 57.067 | 58.773 | 1.00 36.86 | 6 |
| ATOM | 2596 | C | ALA A 32 | | 57.803 | 56.612 | 1.00 43.30 | 6 |
| MOTA | 2597 | Ō | ALA A 32 | | 57.028 | 55.705 | 1.00 42.83 | 8 |
| MOTA | 2598 | N | LYS A 32 | | 58.843 | 56.977 | 1.00 45.56 | 7 |
| ATOM | 2599 | CA | LYS A 32 | 7 29.657 | 59.146 | 56.306 | 1.00 47.23 | 6 |
| ATOM | 2600 | CB | LYS A 32 | 7 29.023 | 60.407 | 56.892 | 1.00 49.59 | 6 |
| ATOM | 2601 | CG | LYS A 32 | 7 28.547 | 60.263 | 58.329 | 1.00 54.63 | 6 |
| ATOM | 2602 | CD | LYS A 32 | 7 28.024 | 61.591 | 58.862 | 1.00 55.89 | 6 |
| ATOM | 2603 | CE | LYS A 32 | 7 27.529 | 61.483 | 60.299 | 1.00 58.28 | 6 |
| MOTA | 2604 | NZ | LYS A 32 | 7 26.304 | 60.644 | 60.426 | 1.00 59.91 | 7 |
| ATOM | 2605 | C | LYS A 32 | 7 29.888 | 59.347 | 54.816 | 1.00 46.97 | 6 |
| MOTA | 2606 | 0 | LYS A 32 | 7 29.090 | 58.913 | 53.990 | 1.00 48.10 | 8 |
| ATOM | 2607 | N | GLU A 32 | | 60.012 | 54.480 | 1.00 44.99 | 7 |
| ATOM | 2608 | CA | GLU A 32 | | 60.264 | 53.091 | 1.00 43.18 | 6 |
| ATOM | . 2609 | CB | GLU A 32 | | 61.326 | 53.027 | 1.00 47.93 | 6 |
| MOTA | 2610 | CG | GLU A 32 | | 62.621 | 53.710 | 1.00 53.65 | 6 |
| MOTA | 2611 | CD | GLU A 32 | | 63.630 | 53.831 | 1.00 55.79 | 6 |
| ATOM | 2612 | | GLU A 32 | | 64.060 | 52.783 | 1.00 58.73 | 8 |
| ATOM | 2613 | OE2 | | | 63.991 | 54.979 | 1.00 58.13 | 8 6 |
| ATOM | . 2614 | C | GLU A 32 | | 58.971 | 52.437 | 1.00 41.56 | 8 |
| ATOM | 2615 | 0 | GLU A 32 | | 58.743 | 51.255 53.211 | 1.00 39.41 1.00 40.64 | 7 |
| MOTA | 2616 | N | LEU A 32 | | 58.123 56.844 | 52.695 | 1.00 36.45 | 6 |
| ATOM | 2617 2618 | CA CB | LEU A 32 LEU A 32 | | 56.032 | 53.801 | 1.00 34.70 | 6 |
| ATOM | 2619 | CG | LEU A 32 | | 54.610 | 53.433 | 1.00 35.69 | 6 |
| ATOM ATOM | 2620 | | LEU A 32 | | 54.642 | 52.359 | 1.00 30.11 | 6 |
| ATOM | 2621 | | LEU A 32 | | 53.926 | 54.683 | 1.00 34.63 | 6 |
| ATOM | 2622 | C | LEU A 32 | | 56.064 | 52.157 | 1.00 35.77 | 6 |
| ATOM | 2623 | ŏ | LEU A 32 | | 55.746 | 50.975 | 1.00 34.94 | 8 |
| ATOM | 2624 | N. | | | 55.770 | 53.029 | 1.00 34.78 | 7 |
| ATOM | 2625 | CA | LEU A 33 | | 55.028 | 52.630 | 1.00 34.95 | 6 |
| ATOM | 2626 | CB | LEU A 33 | | 54.914 | 53.803 | 1.00 30.95 | 6 |
| ATOM | 2627 | CG | LEU A 33 | | 54.115 | 54.991 | 1.00 32.66 | 6 |
| ATOM | 2628 | | LEU A 33 | | 53.904 | 56.022 | 1.00 31.74 | 6 |
| ATOM | 2629 | CD2 | LEU A 33 | 29.674 | 52.769 | 54.509 | 1.00 30.73 | 6 |
| ATOM | 2630 | С | LEU A 33 | | 55.631 | 51.428 | 1.00 37.28 | 6 |
| ATOM | 2631 | 0 | LEU A 33 | 28.395 | 54.901 | 50.557 | 1.00 40.56 | 8 |
| MOTA | 2632 | N | LYS A 33 | 28.806 | 56.957 | 51.383 | 1.00 38.24 | 7 |
| ATOM | 2633 | CA | LYS A 33 | . 28.140 | 57.661 | 50.294 | 1.00 39.59 | 6 |
| MOTA | 2634 | CB | LYS A 33: | . 27.994 | 59.146 | 50.643 | 1.00 42.31 | C |
| ATOM | 3635 | CG | LYS A 333 | . 27.129 | 59.399 | 51.873 | 1.00 45.93 | 6 |
| ATOM | 2636 | CD | LYS A 33: | 27.017 | 60.879 | 52.244 | 1.00 49.72 | 6 |
| ATOM | 2637 | CE | LYS A 33: | 26.271 | 61.698 | 51.193 | 1.00 53.66 | 6 |
| ATOM | 2638 | NZ | LYS A 33: | | 63.114 | 51.640 | 1.00 54.22 | 7 |
| ATOM | 2639 | С | LYS A 33 | | 57.514 | 48.958 | 1.00 41.02 | 6 |
| TOM | 2640 | 0 | LYS A 33: | . 28.220 | 57.485 | 47.904 | 1.00 39.58 | 8 |

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| ATOM | 2641 | N SER A 332 | 30.192 | 57.413 | 49.005 | 1.00 42.69 | 7 |
|--------------|--------------|--------------------------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 2642 | | 30.998 | | | | 6 |
| ATOM | 2643 | | 32.494 | | | | 6 |
| ATOM | 2644 | | 32.862 | | | | |
| ATOM | 2645 | | 30.634 | | | | 8 |
| ATOM | 2646 | | 30.706 | _ | 45.811 | | 6 |
| MOTA | 2647 | | 30.241 | | 47.786 | | 8 |
| ATOM | 2648 | | 29.869 | | | | 7 |
| ATOM | 2649 | | 29.657 | | 47.187 | 1.00 54.86 | 6 |
| ATOM | 2650 | | 29.388 | | 48.246 | | 6 |
| ATOM | 2651 | - | | | 47.559 | 1.00 52.34 | 6 |
| MOTA | 2652 | | 30.892 | | 49.140 | | 6 |
| | 2653 | | 30.766 | | 50.204 | 1.00 60.31 | 6 |
| MOTA MOTA | 2654 | | 28.579 | | 46.396 | 1.00 57.07 | 6 |
| ATOM | 2655 | | 27.572 28.623 | 54.321 | 46.897 | 1.00.55.59 | 8 |
| ATOM | 2656 | | | 53.320 | 45.160 | 1.00 61.14 | 7 |
| | 2657 | | 27.456 | 53.300 | 44.281 | 1.00 65.55 | 6 |
| ATOM | 2658 | | 27.888 | 53.259 | 42.811 | 1.00 69.19 | 6 |
| ATOM | | | 28.784 | 52.073 | 42.491 | 1.00 70.21 | 6 |
| ATOM | 2659 | OD1 ASP A 334 | 29.097 | 51.875 | 41.298 | 1.00 71.47 | 8 |
| MOTA | 2660 | | 29.181 | 51.344 | 43.427 | 1.00 70.91 | 8 |
| MOTA | 2661 | C ASP A 334 | 26.660 | 52.041 | 44.627 | 1.00 65.65 | 6 |
| MOTA | 2662 | O ASP A 334 | 26.797 | 50.996 | 43.990 | 1.00 63.91 | 8 |
| MOTA | 2663 | N PHE A 335 | 25.822 | 52.153 | 45.649 | 1.00 65.73 | 7 |
| ATOM | 2664 | CA PHE A 335 | 25.041 | 51.021 | 46.104 | 1.00 63.44 | 6 |
| MOTA | 2665 | CB PHE A 335 | 24.980 | 51.034 | 47.632 | 1.00 58.05 | 6 |
| MOTA | 2666 | CG PHE A 335 | 24.039 | 50.028 | 48.195 | 1.00 53.82 | 6 |
| ATOM | 2667 | CD1 PHE A 335 | 24.178 | 48.679 | 47.886 | 1.00 52.40 | 6 |
| ATOM | 2668 | CD2 PHE A 335 | 22.978 | 50.429 | 48.989 | 1.00 51.33 | 6 |
| ATOM | 2669 2670 | CE1 PHE A 335 CE2 PHE A 335 | 23.265 | 47.742 | 48.356 | 1.00 52.73 | 6 |
| ATOM | 2671 | | 22.062 | 49.503 | 49.462 | 1.00 53.20 | 6 |
| ATOM | 2672 | CZ PHE A 335 | 22.204 | 48.151 | 49.144 | 1.00 51.76 | 6 |
| MOTA | 2673 | C PHE A 335 | 23.629 | 50.893 | 45.535 | 1.00 65.55 | 6 |
| MOTA | 2674 | O PHE A 335 | 23.230 | 49.810 | 45.097 | 1.00 67.33 | 8 |
| MOTA | 2675 | N GLU A 336 CA GLU A 336 | 22.874 | 51.986 | 45.537 | 1.00 66.47 | 7 |
| MOTA | 2676 | | 21.497 | 51.948 | 45.048 | 1.00 67.43 | 6 |
| ATOM | 2677 | CB GLU A 336 CG GLU A 336 | 21.422 | 51.379 | 43.626 | 1.00 71.79 | 6 |
| MOTA MOTA | 2678 | CD GLU A 336 | 19.982 | 51.245 | 43.116 | 1.00 78.77 | 6 |
| MOTA | 2679 | OE1 GLU A 336 | 19.868 20.232 | 50.505 | 41.789 | 1.00 82.67 | 6 |
| MOTA | 2680 | OE2 GLU A 336 | 19.410 | 49.306 51.126 | 41.734 | 1.00 83.29 | 8 |
| ATOM | 2681 | C GLU A 336 | 20.655 | | 40.801 | 1.00 84.26 | 8 |
| ATOM | 2682 | O GLU A 336 | 20.686 | 51.069 49.840 | 45.971 45.876 | 1.00 64.72 | 6 |
| ATOM | 2683 | N GLU A 337 | 19.901 | 51.710 | 46.858 | 1.00 59.84 1.00 64.47 | 8 7 |
| ATOM | 2684 | CA GLU A 337 | 19.045 | 51.003 | 47.805 | | 6 |
| ATOM | 2685 | CB GLU A 337 | 18.398 | 52.003 | 48.759 | 1.00 65.83 1.00 64.20 | 6 |
| ATOM | 2686 | CG GLU A 337 | 17.753 | 51.370 | 49.964 | 1.00 64.26 | 6 |
| ATOM | 2687 | CD GLU A 337 | 18.774 | 50.εj0 | 50.850 | 1.00 64.26 | 6 |
| ATOM | 2688 | OE1 GLU A 337 | 19.741 | 51.3.2 | 51.261 | 1.00 61.66 | ´ 8 |
| ATOM | 2689 | OE2 GLU A 337 | 18.608 | 49.483 | 51.132 | 1.00 63.64 | 8 |
| ATOM | 2690 | C GLU A 337 | 17.950 | 50.239 | 47.063 | 1.00 67.13 | 6 |
| ATOM | 2691 | O GLU A 337 | 17.269 | 50.807 | 46.205 | 1.00 68.27 | 8 |
| ATOM | 2692 | N PHE A 338 | 17.779 | 48.960 | 47.394 | 1.00 67.22 | 7 |
| ATOM | 2693 | CA PHE A 338 | 16.764 | 48.129 | 46.748 | 1.00 68.05 | 6 |
| ATOM | 2694 | CB PHE A 338 | 16.445 | 46.919 | 47.626 | 1.00 69.68 | 6 |
| ATOM | 2695 | CG PHE A 338 | 15.228 | 46.158 | 47.187 | 1.00 72.35 | 6 |
| ATOM | 2696 | CD1 PHE A 338 | 15.122 | 45.674 | 45.888 | 1.00 72.37 | 6 |
| ATOM | 2697 | CD2 PHE A 338 | 14.172 | 45.941 | 48.074 | 1.00 72.37 | 6 |
| ATOM | 2698 | CE1 PHE A 338 | 13.980 | 44.984 | 45.478 | 1.00 73.81 | 6 |
| ATOM | 2699 | CE2 PHE A 338 | 13.024 | 45.250 | 47.672 | 1.00 73.39 | 6 |
| ATOM | 2700 | CZ PHE A 338 | 12.929 | 44.771 | 46.369 | 1.00 73.26 | 6 |
| ATOM | 2701 | C PHE A 338 | 15.481 | 48.902 | 46.434 | | 6 |
| ATOM | 2702 | O PHE A 338 | 15.286 | 49.367 | 45.310 | 1.00 68.45 1.00 67.92 | 8 |
| ATOM | 2703 | N ASP A 339 | 14.606 | 49.026 | 47.426 | 1.00 68.98 | 7 |
| ATOM | 2704 | CA ASP A 339 | 13.358 | 49.759 | 47.261 | 1.00 70.68 | 6 |
| ATOM | 2705 | CB ASP A 339 | 12.596 | 49.758 | 48.588 | 1.00 70.68 | 6 |
| ATOM | 2706 | CG ASP A 339 | 11.381 | 50.678 | 48.581 | 1.00 72.05 | 6 |
| WI OUT | | CC AGE A 333 | | -0.070 | 30.701 | 1.00 /2.03 | 9 |

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| | 2707 | נתס | ASP A | 330 | 11.548 | 51.893 | 48.320 | 1.00 72.29 | 8 |
|--------------|--------|------|----------|------|--------|----------|--------|---------------------|-----|
| MOTA | | | | | | | | 1.00 71.03 | 8 |
| ATOM | 2708 | OD2 | ASP A | 339 | 10.262 | 50.188 | 48.858 | | |
| ATOM | 2709 | С | ASP A | 339 | 13.715 | 51.183 | 46.853 | 1.00 73.18 | 6 |
| | | | | | 14.407 | 51.884 | 47.592 | 1.00 73.78 | 8 |
| ATOM | 2710 | 0 | ASP A | | | | | | |
| MOTA | 2711 | N | ASP A | 340 | 13.247 | 51.600 | 45.677 | 1.00 76.36 | 7 |
| | 2712 | CA | ASP A | 340 | 13.518 | 52.943 | 45.152 | 1.00 78.34 | 6 |
| MOTA | | | | | | | | 1.00 77.55 | 6 |
| ATOM | 2713 | CB | ASP A | 340 | 12.410 | 53.385 | 44.189 | | |
| ATOM | 2714 | CG | ASP A | 340 | 12.462 | 52.655 | 42.864 | 1.00 78.90 | 6 |
| | | | | | 12.348 | 51,408 | 42.855 | 1.00 78.38 | 8 |
| MOTA | 2715 | | ASP A | | | | | | |
| ATOM | 2716 | OD2 | ASP A | 340 | 12.620 | 53.336 | 41.830 | 1.00 78.74 | 8 |
| | 2717 | С | ASP A | 340 | 13.687 | 54.017 | 46.214 | 1.00 79.51 | 6 |
| MOTA | | | | | | 54.856 | 46.117 | 1.00 80.19 | 8 |
| ATOM | 2718 | 0 | ASP A | | 14.587 | | | | |
| MOTA | 2719 | N | GLU A | 341 | 12.824 | 54.000 | 47.224 | 1.00 79.64 | 7 |
| | | CA | GLU A | 3/11 | 12.922 | 54.998 | 48.271 | 1.00 80.05 | 6 : |
| ATOM | 2720 | | | | | | 47.811 | 1.00 83.75 | 6 |
| ATOM | 2721 | CB | GLU A | 341 | 12.269 | 56.301 | | | |
| MOTA | 2722 | CG | GLU · A | 341 | 12.411 | 57.442 | 48.806 | 1.00 89.02 | 6 |
| | | | GLU A | | 11.756 | 58.724 | 48.328 | 1.00 91.52 | 6 |
| ATOM | 2723 - | CD | | | | | | 1.00 93.33 | 8 |
| ATOM | 2724 | OE1 | GLU A | 341 | 10.515 | 58.738 | 48.175 | | |
| | 2725 | OE2 | GLU A | 341 | 12.484 | 59.716 | 48.102 | 1.00 92.65 | 8 |
| MOTA | | | | | 12.317 | 54.578 | 49.597 | 1.00 77.98 | 6 |
| ATOM | 2726 | С | GLU A | | | | | | |
| MOTA | 2727 | 0 | GLU A | 341 | 11.102 | 54.610 | 49.777 | 1.00 79.82 | 8 |
| | 2728 | N | VAL A | 342 | 13.179 | 54.181 | 50.523 | 1.00 74.49 | 7 |
| MOTA | | | | | 12.745 | 53.793 | 51.859 | 1.00 71.55 | 6 |
| MOTA | 2729 | CA | VAL A | | | | | | |
| MOTA | 2730 | CB | VAL A | 342 | 13.224 | 52.383 | 52.245 | 1.00 72.40 | 6 |
| | 2731 | | VAL A | 342 | 12.672 | 52.004 | 53.610 | 1.00 71.16 | 6 |
| ATOM | | | | | | 51.391 | 51.207 | 1.00 74.35 | 6 |
| MOTA | 2732 | CG2 | VAL A | 342 | 12.797 | | | | |
| ATOM | 2733 | С | VAL A | 342 | 13.454 | 54.778 | 52.766 | 1.00 68.46 | 6 |
| | | ō | VAL A | | 12.952 | 55.154 | 53.829 | 1.00 68.96 | 8 |
| MOTA | 2734 | | | | | 55.184 | 52.311 | 1.00 61.61 | 7 |
| MOTA | 2735 | N | ASP A | 343 | 14.636 | | | | |
| ATOM | 2736 | CA | ASP A | 343 | 15.486 | 56.114 | 53.029 | 1.00 54.91 | 6 |
| | | СВ | ASP A | | 14.678 | 57.303 | 53.543 | 1.00 55.06 | 6 |
| MOTA | 2737 | | | | | | 54.114 | 1.00 54.44 | 6 |
| MOTA | 2738 | CG | ASP A | 343 | 15.556 | 58.390 | | | |
| ATOM | 2739 | OD1 | ASP A | 343 | 15.002 | 59.351 | 54.694 | 1.00 56.20 | 8 |
| | _ | | ASP A | | 16.795 | 58.287 | 53.969 | 1.00 49.32 | 8 |
| ATOM | 2740 | • | | | | | 54.198 | 1.00 50.85 | 6 |
| MOTA | 2741 | С | ASP A | 343 | 16.152 | 55.401 | | | |
| ATOM | 2742 | 0 | ASP A | 343 | 15.557 | 55.209 | 55.257 | 1.00 49.32 | 8 |
| | | N | ARG A | | 17.396 | 55.004 | 53.980 | 1.00 47.84 | 7 |
| MOTA | 2743 | | | | | 54.321 | 54.981 | 1.00 45.34 | 6 |
| ATOM | 2744 | CA | ARG A | 244 | 18.195 | | | | |
| ATOM | 2745 | CB | ARG A | 344 | 18.883 | 53.099 | 54.358 | 1.00 45.00 | 6 |
| | | CG | ARG A | 344 | 17.950 | 51.969 | 53.974 | 1.00 38.03 | 6 |
| ATOM | 2746 | | | | | 51.531 | 55.188 | 1.00 35.83 | 6 |
| ATOM | 2747 | CD | ARG A | 344 | 17.185 | | | | 7 |
| ATOM | 2748 | NE | ARG A | 344 | 16.278 | 50.439 | 54.885 | 1.00 39.20 | |
| | 2749 | CZ | ARG A | | 15.350 | 49.993 | 55.724 | 1.00 39 <i>.</i> 89 | 6 |
| ATOM | | | | | | | 56.917 | 1.00 40.17 | 7 |
| MOTA | 2750 | NH1 | ARG A | 344 | 15.217 | 50.561 | | | |
| ATOM | 2751 | NH2 | ARG A | 344 | 14.566 | 48.976 | 55.375 | 1.00 40.75 | 7 |
| | | С | ARG A | | 19.250 | 55.278 | 55,515 | 1.00 44.72 | 6 |
| ATC I | 2752 | | | | | • | 56.223 | 1.00 46.97 | 8 |
| ATCM | 2753 | 0 | ARG A | | 20.170 | 54.869 | | | 7. |
| ATO.1 | 2754 | N | SER A | 345 | 19.113 | 56.552 | 55.157 | 1.00 45.81 | |
| | 2755 | CA | SER A | | 20.045 | 57.596 | 55.577 | 1.00 43.66 | 6 |
| ATCM | _ | | | | | | 55.115 | 1.00 43.44 | 6 |
| ATOM | 2756 | CB | SER A | | 19.538 | 58.960 | | | |
| ATOM | 2757 | OG | SER A | 345 | 18.292 | 59.260 | 55.722 | 1.00 45.62 | 8 |
| | | c | SERA | 3/15 | 20.258 | 57.627 | 57.089 | 1.00 42.79 | 6 |
| ATOM | 2758 | | SER A | 345 | | | 57.552 | 1.00 42.62 | 8 |
| ATOM | 2759 | 0 | SER A | 345 | 21.364 | 0 | | | |
| | 2760 | N | TYR A | 346 | 19.200 | 57.354 · | 57.851 | 1.00 40.55 | 7 |
| ATOM | | | TYR A | | 19.280 | 57.352 | 59.308 | 1.00 41.05 | 6 |
| ATOM | 2761 | CA | | | | | | 1.00 41.74 | 6 |
| ATOM | 2762 | CB | TYR A | | 17.971 | 56.819 | 59.905 | | |
| | 2763 | CG | TYR A | 346 | 17.668 | 55.355 | 59.630 | 1.00 43.47 | 6 |
| ATOM | | | | | 18.331 | 54.333 | 60.328 | 1.00 44.45 | 6 |
| ATOM | 2764 | CD1 | TYR A | | | | 60.088 | 1.00 41.02 | 6 |
| ATOM | 2765 | CE1 | TYR A | 346 | 18.044 | 52.983 | | | |
| | 2766 | CD2 | TYR A | | 16.710 | 54.988 | 58.682 | 1.00 42.08 | 6 |
| ATOM | | | | | 16.416 | 53.644 | 58.434 | 1.00 40.59 | 6 |
| ATCM | 2767 | CE2 | TYR A | | _ | | | 1.00 41.66 | 5 |
| ATCM | 2768 | CZ | TYR A | 346 | 17.086 | 52.649 | 59.139 | | |
| | 2769 | OH | TYR A | | 16.806 | 51.324 | 58.884 | 1.00 39.60 | 8 |
| ATCM | | | | | 20.466 | 56.517 | 59.796 | 1.00 42.92 | 6 |
| ATCM | 2770 | С | TYR A | | | | | 1.00 42.65 | 8 |
| ATCM | 2771 | 0 | TYR A | 346 | 21.101 | 56.844 | 60.799 | 1.00 44.00 | |
| | | N | MET A | 347 | 20.757 | 55.443 | 59.067 | 1.00 44.59 | 7 |
| <u>ኋጥ</u> ርዝ | 2772 | TA . | The same | _ | | | _ | | |

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Figure 17-43

| ATOM | 2773 | C | MET A 347 | | 21.85 | 9 54.546 | 59.388 | 1.00 45.89 | 6 |
|--------|--------|-----|-------------|---|--------|----------|--------|-------------|-----|
| ATOM | 2774 | CE | MET A 347 | | 21.95 | | | | |
| ATOM | | C | | | 20.72 | | | | 6 |
| | | SI | | | | | | | 6 |
| MOTA | 2776 | | | | 21.06 | | | | 16 |
| ATOM | 2777 | CE | | | 21.54 | 5 52.237 | 55.676 | 1.00 44.55 | б |
| ATOM - | 2778 | С | MET A 347 | | 23.188 | 55.286 | 59.404 | 1.00 48.47 | 6 |
| MOTA | 2779 | 0 | MET A 347 | | 24.129 | 54.888 | | | 8 |
| ATOM | 2780 | N | LEU A 348 | | 23.25 | | | | 7 |
| ATOM | 2781 | CA | | | 24.458 | | | 1.00 49.03 | |
| - | 2782 | CE | | | | _ | | | 6 |
| ATOM | | | | | 24.355 | | | | 6 |
| MOTA | 2783 | CG | | | 24.280 | | | 1.00 44.47 | 6 |
| MOTA | 2784 | CD | 1 LEU A 348 | | 23.908 | 3 58.476 | 54.859 | 1.00 43.62 | 6 |
| MOTA | 2785 | CD | 2 LEU A 348 | - | 25.618 | 3 56.757 | 55.565 | | 6 |
| ATOM | 2786 | С | LEU A 348 | | 24.644 | 58.049 | | 1.00 49.33 | 6 |
| ATOM | 2787 | 0 - | LEU A 348 | | 25.765 | | | 1.00 49.78 | |
| ATOM | 2788 | N | GLU A 349 | | 23.537 | | | | 8 |
| _ | 2789 | CA | | | | | | 1.00 48.34 | 7 |
| ATOM | | | | | 23.591 | | | 1.00 49.24 | 6 |
| ATOM | 2790 | CB | | | 22.198 | | 61.811 | 1.00 48.36 | 6 |
| ATOM | 2791 | CG | | | 21.628 | 60.584 | 60.607 | 1.00 45.52 | 6 |
| ATOM | 2792 | CD | GLU A 349 | | 22.598 | 61.619 | 60.065 | 1.00 42.94 | 6 |
| ATOM | 2793 | OE: | 1 GLU A 349 | | 22.934 | 62.560 | 60.812 | 1.00 40.82 | 8 |
| ATOM | 2794 | OE | 2 GLU A 349 | | 23.028 | | 58.900 | 1.00 38.30 | |
| ATOM | 2795 | C | GLU A 349 | | 24.119 | | | | 8 |
| | 2796 | ŏ | GLU A 349 | | | | 62.745 | 1.00 48.32 | 6 |
| ATOM | | | | | 25.226 | | 63.219 | 1.00 47.87 | 8 |
| MOTA | 2797 | N | THR A 350 | | 23.325 | | 63.248 | 1.00 48.97 | 7 |
| ATOM | 2798 | CA | THR A 350 | | 23.744 | | 64.398 | 1.00 50.70 | 6 |
| MOTA | 2799 | CB | THR A 350 | | 22.558 | 56.596 | 65.342 | 1.00 51.02 | 6 |
| MOTA | 2800 | OG: | | | 22.071 | 57.865 | 65.803 | 1.00 49.11 | 8 |
| ATOM | 2801 | CG2 | 2 THR A 350 | | 22.983 | 55.763 | 66.537 | 1.00 51.58 | 6 |
| MOTA | 2802 | С | THR A 350 | | 24.361 | | 63.954 | 1.00 49.56 | 6 |
| MOTA | 2803 | 0 | THR A 350 | | 23.979 | 54.947 | 62.923 | 1.00 50.55 | 8 |
| ATOM | 2804 | N | LEU A 351 | | 25.333 | 55.028 | | | |
| | 2805 | CA | LEU A 351 | | | | 64.725 | 1.00 46.88 | 7 |
| ATOM | | | | | 26.018 | 53.781 | • | 1.00 45.35 | 6 |
| MOTA | 2806 | CB | LEU A 351 | | 27.342 | 53.726 | 65.185 | 1.00 47.05 | 6 |
| MOTA | 2807 | CG | LEU A 351 | | 28.257 | 52.502 | 65.072 | 1.00 49.54 | 6 |
| ATOM | 2808 | CD1 | . LEU A 351 | | 29.575 | 52.777 | 65.766 | 1.00 51.50 | 6 |
| MOTA | 2809 | CD2 | LEU A 351 | | 27.603 | 51.302 | 65.692 | 1.00 48.35 | 6 |
| ATOM | 2810 | С | LEU A 351 | | 25.145 | 52.584 | 64.772 | 1.00 44.79 | 6 |
| MOTA | 2811 | 0 | LEU A 351 | | 25.131 | 51.578 | 64.061 | 1.00 41.45 | 8 |
| ATOM . | 2812 | N | LYS A 352 | | 24.420 | 52.711 | 65.880 | | 7 |
| ATOM | 2813 | CA | LYS A 352 | | 23.531 | | | 1.00 45.27 | |
| | 2814 | CB | | | | 51.662 | 66.375 | 1.00 44.62 | 6 |
| MOTA | | | LYS A 352 | | 23.764 | 51.464 | 67.873 | 1.00 42.23 | 6 |
| ATOM | 2815 | CG | LYS A 352 | | 25.197 | 51.075 | 68.187 | 1.00 44.94 | 6 |
| ATOM | 2816 | CD | LYS A 352 | | 25.572 | 51.262 | 69.650 | 1.00 46.80 | 6 |
| MOTA | 2817 | CE | LYS A 352 | | 24.765 | 50.389 | 70.581 | 1.00 45.79 | 6 |
| ATOM | 2818 | NZ | LYS A 352 | | 25.236 | 50.586 | 71.975 | 1.00 47.31 | 7 |
| ATOM | 2819 | С | LYS A 352 | | 22.096 | 52.087 | 66.116 | 1.00 45.12 | 6 |
| MOTA | 2820 | 0 | LYS A 352 | | 21.837 | 53.236 | 65.756 | 1.00 47.07 | 8 |
| ATOM | | N | ASP A 353 | | 21.162 | 51.161 | 66.285 | 1.00 44.62 | 7 . |
| ATOM | | CA | ASP A 353 | | 19.761 | 51.474 | 66.060 | | |
| | • | CB | ASP A 353 | | | | | 1.00 46.43 | 6 |
| MOTA | | | | | 19.302 | 50.943 | | 1.00 49.38 | 6 |
| MOTA | | CG | ASP A 353 | | 19.813 | 49.546 | 64.396 | .1.00 51.52 | 6 |
| ATOM | | OD1 | | | 21.028 | 49.396 | 64.158 | 1.00 55.36 | 8 |
| ATOM | 2826 | OD2 | ASP A 353 | | 19.005 | 48.596 | 64.398 | 1.00 52.35 | 8 |
| MOTA | | С | ASP A 353 | | 18.841 | 50.968 | 67.165 | 1.00 45.90 | 6 |
| ATOM | | 0 | ASP A 353 | | 19.152 | 50.001 | 67.854 | 1.00 45.98 | 8 |
| ATOM | | N | PRO A 354 | | 17.687 | 51.629 | 67.348 | 1.00 45.86 | 7 |
| ATOM | | מכ | PRO A 354 | | 17.162 | 52.775 | | | |
| | | | | | | | 66.587 | 1.00 45.36 | 6 |
| ATOM | | CA | PRO A 354 | | 16.723 | 51.243 | 68.378 | 1.00 45.52 | 6 |
| MOTA | | CB | PRO A 354 | | 15.585 | 52.245 | 68.159 | 1.00 44.77 | 6 |
| MOT. | | CG | PRO A 354 | | 15.681 | 52.513 | 66.664 | 1.00 45.06 | 6 |
| ATOM | 2834 (| 2 | PRO A 354 | | 16.277 | 49.804 | 68.188 | 1.00 44.13 | 6 |
| ATOM | |) | PRO A 354 | | 16.352 | 49.271 | 67.078 | 1.00 42.90 | 8 |
| | | J | TRP A 355 | | 15.821 | 49.174 | 69.267 | 1.00 42.77 | 7 |
| ATOM | | À | TRP A 355 | | 15.358 | 47.801 | 69.168 | 1.00 43.35 | |
| | | | TRP A 355 | | 14.982 | 47.225 | | 1.00 47.11 | 6 |
| ATCM | , oco | . D | A 333 | | 14.304 | 41.223 | 70.539 | 1.00 47.11 | 6 |
| | | | | | | | | • | _ |

| ATOM | 2839 | CG | TRP A 3 | 55 | 16.168 | 46.752 | 71.322 | 1.00 52.43 | 6 |
|--------------|--------------|-----|----------------------|--------|------------------|------------------|------------------|--------------------------|---------|
| MOTA | 2840 | | | | 16.574 | 45.391 | 71.519 | 1.00 53.15 | 6 |
| ATOM | 2841 | | | | 17.789 | 45.416 | 72.238 | 1.00 54.97 | 6 |
| MOTA | 2842 | | | | 16.031 | | 71.155 | 1.00 53.39 | 6 |
| ATOM | 2843 | | | | 17.125 | 47.526 | 71.916 | 1.00 54.39 | 6 |
| MOTA | 2844 | | | | 18.103 | 46.731 | 72.468 | 1.00 57.31 | 7 |
| ATOM | 2845 | | | | 18.469 | 44.249 | 72.602 | 1.00 54.97 | 6 |
| ATOM | 2846 | | | | 16.706 | 42.995 | 71.518 | 1.00 55.77 | |
| MOTA | 2847 | | 2 TRP A 3 | | 17.913 | 43.052 | 72.234 | | 6 |
| ATOM | 2848 | c. | TRP A 3 | | 14.177 | 47.690 | 68.230 | 1.00 54.84 | 6 |
| MOTA | 2849 | | TRP A 3 | | 13.508 | 48.677 | 67.915 | 1.00 41.94 | 6 |
| ATOM | 2850 | N | ARG A 3 | | 13.942 | 46.471 | | 1.00 41.39 | 8 |
| ATOM | 2851 | CA | | | 12.855 | 46.185 | 67.775 | 1.00 38.60 | 7 |
| ATOM | 2852 | CB | ARG A 3 | | 13.413 | | 66.866 | 1.00 36.55 | 6 |
| ATOM | 2853 | CG | ARG A 3 | | 14.120 | 46.044 | 65.451 | 1.00 35.06 | 6 |
| MOTA | 2854 | CD | | | 14.969 | 47.308 | 64.976 | 1.00 32.47 | 6 |
| | 2855 | NE | ARG A 35 | | | 47.082 | 63.733 | 1.00 29.54 | 6 |
| ATOM | 2856 | | | | 15.600 16.514 | 48.323 | 63.296 | 1.00 28.91 | 7 |
| ATOM | | CZ | ARG A 35 | | | 48.403 | 62.335 | 1.00 30.60 | 6 |
| ATOM | 2857 | NH. | | | 16.916 | 47.305 | 61.702 | 1.00 33.52 | 7 |
| MOTA | 2858 | NH | | | 17.020 | 49.582 | 61.996 | 1.00 30.10 | 7 |
| ATOM | 2859 | C | ARG A 35 | | 12.270 | 44.879 | 67.361 | 1.00 36.01 | 6 |
| ATOM | 2860 | 0 | ARG A 35 | | 12.447 | 43.831 | 66.742 | 1.00 38.38 | 8 |
| ATOM | 2861 | N | GLY A 35 | | 11.587 | 44.949 | 68.499 | 1.00 36.04 | 7 |
| ATOM | 2862 | CA | GLY A 35 | | 11.001 | 43.758 | 69.085 | 1.00 36.08 | 6 |
| ATOM | 2863 | C | GLY A 35 | | 9.514 | 43.596 | 68.851 | 1.00 34.51 | 6 |
| MOTA | 2864 | 0 | GLY A 35 | | 8.943 | 44.196 | 67.943 | 1.00 36.77 | 8 |
| ATOM | 2865 | N | GLY A 35 | | 8.892 | 42.772 | 69.687 | 1.00 36.04 | . 7 |
| MOTA | 2866 | CA | GLY A 35 | | 7.466 | 42.506 | 69.593 | 1.00 32.26 | ` 6 |
| ATOM | 2867 | C | GLY A 35 | | 7.106 | 41.263 | 70.385 | 1.00 29.85 | 6 |
| ATOM | 2868 | 0 | GLY A 35 | | 7.832 | 40.839 | 71.288 | 1.00 28.86 | 8 |
| MOTA | 2869 | N | GLU A 35 | | 5.975 | 40.667 | 70.055 | 1.00 30.88 | 7 |
| MOTA | 2870 | CA | GLU A 35 | | 5.550 | 39.455 | 70.743 | 1.00 32.58 | . 6 |
| ATOM | 2871 | CB | GLU A 35 | | 4.034 | 39.289 | 70.604 | 1.00 38.60 | 6 |
| ATOM | 2872 | CG | GLU A 35 | | 3.230 | 40.435 | 71.222 | 1.00 47.44 | 6 |
| ATOM | 2873 | CD | GLU A 35 | | 1.957 | 40.762 | 70.445 | 1.00 50.93 | 6 |
| MOTA | 2874 | | GLU A 35 | | 1.123 | 39.852 | 70.221 | 1.00 52.13 | 8 |
| ATOM | 2875 2876 | C | GLU A 35 GLU A 35 | | 1.798 | 41.942 | 70.061 | 1.00 51.03 | 8 |
| ATOM | 2877 | 0 | GLU A 35 | | 6.250 6.790 | 38.275 | 70.091 | 1.00 28.29 | 6 |
| MOTA | 2878 | N | VAL A 36 | | 6.263 | 38.382 | 68.997 | 1.00 27.88 | 8 |
| MOTA | 2879 | CA | VAL A 36 | | 6.859 | 37.147 | 70.772 | 1.00 27.97 | 7 |
| MOTA | 2880 | CB | VAL A 36 | | 7.673 | 35.957 35.168 | 70.193 | 1.00 25.86 | 6 |
| ATOM | 2881 | | VAL A 36 | | 8.155 | 33.849 | 71.237 70.641 | 1.00 22.02 | 6 |
| ATOM ATOM | 2882 | | VAL A 36 | | 8.850 | 36.009 | 71.698 | 1.00 19.45 1.00 17.88 | 6 |
| ATOM | 2883 | C | VAL A 36 | | 5.703 | 35.099 | 69.670 | | 6 |
| ATOM | 2884 | c | VAL A 36 | | 4.842 | 34.655 | 70.440 | 1.00 28.04 1.00 27.34 | 6 |
| ATOM | 2885 | N | ARG A 36 | | 5.663 | 34.898 | 68.358 | 1.00 27.70 | 8. 7 |
| ATOM - | 2886 | C., | ARG A 36 | | 4.612 | 34.091 | 67.765 | 1.00 27.70 | 6 |
| ATOM | 2887 | CB | ARG A 36 | | 4.693 | 34.164 | 66.242 | 1.00 32.30 | 6 |
| MOTA | 2888 | CG | ARG A 36 | | 4.243 | 35.504 | 65.687 | 1.00 32.30 | 6 |
| ATOM | 2889 | CD | ARG A 36: | | | 35.653 | 64.201 | 1.00 40.09 | 6 |
| | 2890 | NE | ARG A 363 | | 5.974 | | 63.961 | | |
| MOTA | 2891 | CZ | ARG A 36 | | 6.514 | 35.812 | 62.763 | 1.00 38.77 | 7 |
| ATOM | | | _ | | | 35.989 | | 1.00 39.21 | 6 |
| ATOM | 2892 | NH1 | | | 5.748 | 36.027 | 61.685 | 1.00 40.79 | 7 |
| ATOM | 2893 | NH2 | ARG A 361 | | 7.822 | 36.145 | 62.643 | 1.00 42.94 | 7 |
| ATOM | 2894 | C | | | 4.689 | 32.638 | 68.222 | 1.00 35.65 | 6 |
| MOTA | 2895 | 0 | ARG A 361 | L) | 5.768 | 32.097 | 68.471 | 1.00 37.08 | 8 |
| ATOM | 2896 | N | LYS A 362 | | 3.526 | 32.017 | 68.347 | 1.00 37.80 | 7 |
| MOTA | 2897 | CA | LYS A 362 | | 3.436 | 30.626 | 68.757 | 1.00 39.91 | ,6 6 |
| MOTA | 2898 | CB | LYS A 362 | | 1.982 | 30.152 | 68.648 | 1.00 43.43 | |
| MOTA | 2899 | CG | LYS A 362 | | 1.014 | 30.803 | 69.640 | 1.00 45.11 | 6 |
| ATOM | 2900 | CD | LYS A 362 | | 1.117 | 32.346 | 69.673 | 1.00 49.43 | 6 |
| MOTA | 2901 | CE | LYS A 362 | | 0.813 | 33.022 | 68.327 | 1.00 45.02 | 6 |
| ATOM | 2902 | NZ | LYS A 362 | | 0.962 | 34.509 | 68.422 | 1.00 41.08 | 7 |
| ATOM | 2903 | С | LYS A 362 | | 4.320 | 29.809 | 67.831 | 1.00 39.25 | 6 |
| ATOM | 2904 | 0 | LYS A 362 | • | 4.953 | 28.835 | 68.248 | 1.00 35.45 | 8 |

| | • |
|---|--|
| ATOM 2905 N GLU A 363 | 4.358 30.229 66 568 1 00 41 40 |
| ATOM 2906 CA GLU A 363 | 5 1.13 7 |
| ATOM 2907 CB GLU A 363 | 3.147 29.554 65.539 1.00 43.96 6 |
| | 3.223 30.416 64.278 1.00 45 90 6 |
| 00 0H0 11 305 | 3.03/ 30 8/6 63 7/1 1 00 00 00 |
| ATOM 2909 CD GLU A 363 | 4.045 31 738 62 507 1 00 50.00 |
| ATOM 2910 OE1 GLU A 363 | 4.571 31 224 61 404 1.00 34.11 6 |
| ATOM 2911 OE2 GLU A 363 | 2 645 22 24 24 1.00 53.90 8 |
| ATOM 2912 C GLU A 363 | 5 FEO 0 1202 1.00 30,03 B |
| ATOM 2913 O GLU A 363 | 7 000 20 100 44.39 6 |
| 020 11 303 | 7.002 28.169 65.989 1.00 41.48 8 |
| - | /·+03 30.360 66.540 1 00 37 37 = |
| | 0.335 10 291 67 064 4 66 |
| ATOM 2916 CB VAL A 364 | 9.038 31 696 67 460 |
| ATOM 2917 CG1 VAL A 364 | 10.444 31 500 60 043 1.00 36.88 6 |
| ATOM 2918 CG2 VAL A 364 | 0.010 1.00 3/.// 6 |
| ATOM 2919 C VAL A 364 | 1.00 34.78 6 |
| ATOM 2920 O VAL A 364 | 1.00 33.01 |
| ATOM 2921 N LYS A 365 | 3.022 28.614 68.379 1.00 31.55 B |
| | 7.004 29.409 69.165 1.00 32 61 2 |
| | 7.674 28 567 70 363 |
| ATOM 2923 CB LYS A 365 | 6.598 29 010 71 250 1 00 |
| ATOM 2924 CG LYS A 365 | C 00C 00 JU-1J 0 |
| ATOM 2925 CD LYS A 365 | 5.837 30 781 72 005 1.00 36.02 6 |
| ATOM 2926 CE LYS A 365 | 5 20 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM 2927 NZ LYS A 365 | 70.505 1.00 41.58 6 |
| ATOM 2928 C LYS A 365 | 3.191 32.611 74.585 1.00 44.29 7 |
| ATOM 2929 O LYS A 365 | 7.432 27.114 70.007 1.00 30.32 6 |
| | 0.195 20.237 70.442 1.00 31 32 0 |
| | 6.427 26.863 69.209 1.00 29.85 7 |
| 1102 21 300 | 6.115 25 500 60 002 + 00 5 |
| ATOM 2932 CB ASP A 366 | 4.948 25 522 67 818 1 88 32.07 |
| ATOM 2933 CG ASP A 366 | 3 344 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 |
| ATOM 2934 OD1 ASP A 366 | 3 |
| ATOM 2935 OD2 ASP A 366 | 1.00 40.16 8 |
| ATOM 2936 C ASP A 366 | 7 |
| ATOM 2937 O ASP A 366 | 7.343 24.866 68.161 1.00 33.07 6 |
| 11 300 | 7.753 23.763 68.540 1.00 32 64 8 |
| | 7.932 25.565 67.193 1.00 31.89 7 |
| 11 307 | 9.088 25.045 66.490 1.00 31.17 6 |
| ATOM 2940 CB THR A 367 | 9.712 26.070 65.572 |
| ATOM 2941 OG1 THR A 367 | 0 707 |
| ATOM 2942 CG2 THR A 367 | 1.00 34.37 8 |
| ATOM 2943 C THR A 367 | 04.723 1.00 33.55 6 |
| ATOM 2944 O THR A 367 | 10 505 |
| ATOM 2945 N LEU A 368 | 10 30.02 8 |
| ATOM 2946 CA LEU A 368 | 7 |
| ATOM 2947 CB LEU A 368 | 11.582 25.264 69.288 1.00 32.87 6 |
| | 11.848 26.478 70.179 1.00 27 73 6 |
| | 12.88/ 27.449 69.588 1.00 29 05 6 |
| | 14.260 26.777 69.541 1.00 23.05 6 |
| ATOM 2950 CD2 LEU A 368 | |
| ATOM 2951 C LEU A 368 | 11 157 24 053 30 103 |
| ATOM 2952 O LEU A 368 | 11 910 22 077 70 217 |
| ATOM 2953 N GLU A 369 | 70.217 1.00 35.18 8 |
| ATOM 2954 CA GLU A 369 | 1.00 37.36 |
| ATOM 2955 CB GLU A 369 | 6 |
| ATOM 2956 CG GLU A 369 | 7.956 23.216 71.770 1.00 42.07 6 |
| ATOM 2957 CD GLU A 369 | 7.722 24.460 72.617 1.00 48.51 6 |
| | 6.281 24.616 73.067 1.00 51.93 6 |
| | 5./// 23.724 73.782 1.00 52 g/ g |
| ATOM 2959 OE2 GLU A 369 | 5.652 25.636 72.710 1.00 58 33 0 |
| ATOM 2960 C GLU A 369 | 9 633 21 672 72 72 72 |
| ATOM 2961 O GLU A 369 | 10 087 20 604 71 206 |
| ATOM 2962 N LYS A 370 | 9 309 21 652 60 414 |
| ATOM 2963 CA LYS A 370 | 9 497 20 443 60 626 1.00 39.65 |
| ATOM 2964 CB LYS A 370 | 2.00 30.20 |
| ATOM 2965 CG LYS A 370 | 1.00 40.63 h |
| ATOM 2966 CD LYS A 370 | 7.675 20.597 66.854 1.00 44.49 6 |
| | |
| 3TOM 2967 CE ++ 224 | |
| ATOM 2967 CE LYS A 370 | 6.052 20.023 65.015 1.00 54.28 6 |
| ATOM 2968 NZ LYS A 370 | 6.052 20.023 65.015 1.00 54.28 6 5.890 19.679 63.574 1.00 55.44 7 |
| ATOM 2968 NZ LYS A 370 ATOM 2969 C LYS A 370 | 6.052 20.023 65.015 1.00 54.28 6 5.890 19.679 63.574 1.00 55.44 7 |
| ATOM 2968 NZ LYS A 370 | 6.052 20.023 65.015 1.00 54.28 6 5.890 19.679 63.574 1.00 55.44 7 |

| 3 mov . | 2971 | N | ALA | ъ 3 | 71 | 11.8 | 227 | 20.944 | 68.325 | 1.00 | 37.78 | 7 |
|---------|------|-----|----------------|------------|--------------|-------|------|-----------------|--------|------|-------|-----|
| ATOM | | | | | | | | 20.704 | 68.340 | 1.00 | | 6 |
| ATOM | 2972 | CA | ALA | AЗ | 71 | 13.2 | | | | | | |
| ATOM | 2973 | CB | ALA | А3 | 71 | 14.0 | 007 | 22.030 | 68.200 | 1.00 | | 6 |
| | 2974 | С | ALA | 7 3 | 71 | 13.7 | 719 | 19.972 | 69.603 | 1.00 | 35.42 | 6 |
| MOTA | | | | | | | | | 69.525 | 1.00 | | 8 |
| ATOM | 2975 | 0 | ALA | A 3 | /1 | 14.4 | | 18.964 | | | | |
| MOTA | 2976 | N | ALA | А3 | 72 | 13.3 | 317 | 20.478 | 70.766 | 1.00 | 33.96 | 7 |
| | | | ALA | | | 13.6 | 595 | 19.848 | 72.024 | 1.00 | 32.22 | 6 |
| ATOM | 2977 | CA | | | | | | | 73.165 | 1.00 | | 6 |
| ATOM | 2978 | CB | ALA | AЗ | 72 | 12.9 | 140 | 20.486 | | | | |
| | 2979 | С | A.I.A | E. A | 72 | 13.3 | 372 | 18.362 | 71.953 | 1.00 | 31.75 | 6 |
| MOTA | | | | | | 14.1 | | 17.517 | 72.338 | 1.00 | 31.56 | 8 |
| ATOM | 2980 | 0 | ALA | | | | | | | | | |
| ATOM | 2981 | N | ALA | ΑЗ | 73 - | 12.1 | L87 | 18.059 | 71.432 | 1.00 | | 7 . |
| | 2982 | CA | ALA | ΣД | 73 | 11.7 | 710 | 16.684 | 71.305 | 1.00 | 32.32 | 6 |
| MOTA | | | | | | | | 16.689 | 71.103 | 1.00 | 30 18 | 6 |
| MOTA | 2983 | CB | ALA | | | 10.2 | | | | | | |
| MOTA | 2984 | С | ALA | ΑЗ | 73 | 12.3 | 385 | 15.921 | 70.172 | 1.00 | | 6 |
| | 2985 | വ വ | ALA | F A | 73 | 13.0 | 78 | 14.926 | 70.468 | 1.00 | 35.87 | 8 |
| MOTA | | | | | | | | 16.320 | 69.003 | 1.00 | 34 11 | 8 |
| ATOM | 2986 | OT2 | YTY. | | | 12.2 | | | | | | |
| ATOM | 2987 | ZN | ZN | Z 9 | 51 | 22.6 | 593 | 34.497 | 53.990 | 1.00 | | 6 |
| | 2988 | | WAT | | 1 | 35.6 | 554 | 44.211 | 49.416 | 1.00 | 9.27 | 8 |
| MOTA | | | | | | | | 33.130 | 53.069 | 1.00 | 21 27 | 8 |
| ATOM | 2989 | OH2 | WAT | S | 2 | 24.4 | | | | | | |
| ATOM | 2990 | OH2 | WAT | S | 3 | 22.1 | 124 | 30.277 | 59.314 | 1.00 | | 8 |
| | 2991 | OH2 | WAT | S | 4 | 13.8 | 339 | 20.611 | 75.741 | 1.00 | 27.94 | 8 |
| MOTA | | | | | | 34.0 | | 41.903 | 46.522 | 1.00 | 44.54 | 8 |
| ATOM | 2992 | | TAW | | 5 | | | | | | | 8 |
| MOTA | 2993 | OH2 | WAT | S | 6 | 15.0 | 339 | 42.130 | 55.781 | | 23.79 | |
| | 2994 | OH2 | WAT | S | 7 | 32.7 | 737 | 41.397 | 75.900 | 1.00 | 15.80 | 8 |
| ATOM | | | | | 8 | 11.3 | | 22.606 | 58.814 | 1 00 | 23.37 | 8 |
| ATOM | 2995 | | WAT | | | | | | | | 29.93 | 8 |
| ATOM | 2996 | OH2 | \mathbf{WAT} | S | 9 | 13.9 | 909 | 18.160 | 65.105 | | | |
| ATOM | 2997 | OH2 | WAT | S | 10 | 29.6 | 555 | 56.108 | 58.029 | 1.00 | 50.54 | 8 |
| | | | | | 11 | 45.4 | | 17.964 | 51.885 | 1.00 | 9.28 | 8 |
| ATOM | 2998 | | WAT | | | | | | | | 32.78 | 8 |
| ATOM | 2999 | OH2 | WAT | S | 12 | 21.8 | | 35.873 | 34.515 | | | |
| ATOM | 3000 | OH2 | WAT | S | 13 | 43.5 | 504 | 35.670 | 33.779 | | 28.85 | 8 |
| | 3001 | | WAT | | 14 | 2.0 | 054 | 37.997 | 68.430 | 1.00 | 40.53 | 8 |
| ATOM | | | | | | | | 28.024 | 55.966 | | 21.42 | .8 |
| ATOM | 3002 | OH2 | \mathbf{WAT} | S | 15 | 49. | | | | | | |
| ATOM | 3003 | OH2 | WAT | S | 16 | 47.9 | 503 | 32.289 | 34.336 | | 26.13 | 8 |
| | 3004 | | WAT | | 17 | 6.3 | 101 | 26.102 | 64.434 | 1.00 | 21.69 | 8 |
| ATOM | | | | | _ | 10. | | 46.748 | 45.836 | 1 00 | 15.79 | 8 |
| ATOM | 3005 | | TAW | | 18 | | | | | | 16.68 | 8 |
| ATOM | 3006 | OH2 | WAT | S | 19 | 9.: | 146 | 16.861 | 61.441 | | _ | |
| | 3007 | | TAW | | 20 | 5.6 | 684 | 34.080 | 76.599 | 1.00 | 37.53 | 8 |
| ATOM | | | | | | 14.8 | | 33.163 | 49.117 | 1.00 | 34.17 | 8 |
| MOTA | 3008 | | TAW | | 21 | | | | | | 35.64 | 8 |
| ATOM | 3009 | OH2 | TAW | s | 22 | 43. | | 40.839 | 36.825 | | | |
| ATOM | 3010 | OH2 | TAW | S | 23 | 0.5 | 516 | 2 7 .705 | 69.174 | 1.00 | 21.02 | 8 |
| | | | WAT | | 24 | 41.2 | 270 | 25.444 | 29.717 | 1.00 | 29.80 | 8 |
| ATOM | 3011 | | | | | | | | 54.584 | 3 00 | 27.92 | 8 |
| ATOM | 3012 | | WAT | | 25 | 17. | | 29.142 | | | | 8 |
| ATOM | 3013 | OH2 | WAT | S | 26 | 21. | 512 | 60.572 | 56.912 | | 16.77 | |
| | 3014 | | WAT | | 27 | 21.2 | 211· | 33.582 | 48.347 | 1.00 | 23.93 | 8 |
| MOTA | | | | | | 47. | | 24.638 | 56.619 | 1.00 | 23.73 | 8 |
| ATOM | 3015 | OH2 | TAW | | 28 | | | | | | | 8 |
| MOTA | 3016 | OH2 | WAT | S | 25 | 44. | 624 | 50.302 | 58.154 | | 16.79 | |
| | 3017 | OH2 | WAT | S | 3 <i>`</i> ` | 31.0 | 096 | 16.437 | 51.311 | 1.00 | 26.61 | 8 |
| MOTA | | | WAT | | 31 | 39. | 937 | 38.833 | 55.145 | 1.00 | 32.28 | 8 |
| ATOM | 3018 | | | | | | | _ | 63.704 | | 22.94 | 8 |
| MOTA | 3019 | OH2 | WAT | S ' | 32 | 11.0 | | 43.601 | | | | |
| ATOM | 3020 | OH2 | WAT | S | 33 | 49. | 899 | 23.474 | 53.058 | | 26.85 | 8 |
| | | Ona | WAT | ς . | 34 | 34.6 | 624 | 17.734 | 32.228 | 1.00 | 21.18 | 8 |
| MOTA | 3021 | UNZ | 1121 | 2 | | 26.5 | | 15.913 | 62.444 | 1.00 | 27.01 | 8 |
| ATOM | 3022 | OH2 | WAT | S | 35 | | | | | | | |
| MOTA | 3023 | OH2 | WAT | S | 36 | 8.8 | 893 | 28.686 | 63.905 | | 27.68 | 8 |
| | | | WAT | | 37 | 23.3 | 381 | 26.634 | 43.532 | 1.00 | 24.42 | 8 |
| MOTA | 3024 | | | | | | | | 65.270 | | 34.86 | 8 |
| ATOM | 3025 | | TAW | | 38 | 48. | | 27.990 | | | | 8 |
| ATOM | 3026 | OH2 | WAT | Ş | 39 | 43.3 | 28 د | 28.410 | 74.379 | | 25.68 | |
| | 3027 | | WAT | | 40 | 42.5 | 904 | 18.967 | 70.272 | 1.00 | 29.45 | 8 |
| ATOM | • | | | | | 20. | | 53.828 | 50.298 | | 22.35 | 8 |
| ATOM | 3028 | | TAW | | 41 | | | | | | 23.32 | 8 |
| ATOM | 3029 | | WAT | | 42. | 13.: | | 38.921 | 48.404 | | | |
| | 3030 | | WAT | | 43 | 9 _ ' | 787 | 46.265 | 60.012 | | 33.51 | 8 |
| ATOM | | | | | | 36. | | 30.416 | 51.377 | 1,00 | 47.75 | 8 |
| ATOM | 3031 | | WAT | | 44 | | | | | 1 00 | 50.96 | 8 |
| ATOM | 3032 | OH2 | WAT | S | 45 | 14. | | 48.131 | 42.151 | 1.00 | 20.50 | |
| | 3033 | | TAW | | 46 | 54. | 162 | 48.194 | 60.971 | 1.00 | 22.66 | 8 |
| ATOM | | | | | 47 | 38. | | 61.290 | 63.509 | 1.00 | 33.73 | 8 |
| atom | 3034 | | WAT | _ | | | | | 33.130 | 1:00 | 35.80 | 8 |
| MOTA | 3035 | OH2 | WAT | S | 48 | 29. | | 18.112 | | | | 8 |
| ATOM | 3036 | OH2 | WAT | S | 49 | 31. | 879 | 50.673 | 44.528 | 1.00 | 24.39 | o |
| ATOM | | | | • | | | | | _ | • | | |
| | | | | | | | | | | | | |

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Figure 17-47

| ATOM | 1 3037 OH2 WAT S 50 | 39.863 14.629 64.307 1.00 24 19 |
|------|---------------------|--|
| ATOM | | 1.00 24.19 |
| ATOM | | 10 0 10 10 10 10 10 10 10 10 10 10 10 10 |
| ATOM | | 1.00 36.38 |
| ATOM | | 50.802 29.649 52.495 1.00 31.04 |
| ATOM | | 49.540 35.532 71.585 1.00 20 96 |
| ATOM | | 6-88/ 23.426 64.961 1.00 17 40 c |
| | | 25.698 39.891 37.674 1.00 51.51 |
| ATOM | | 47 498 44 101 55 303 1 00 2= - |
| ATOM | | 44 hb 1 14 733 46 000 2 00 |
| ATOM | | 21 912 21 320 70 222 1 00 24 32 |
| MOTA | 3047 OH2 WAT S 60 | 27 290 21 016 27 220 1 00 25.36 |
| MOTA | 3048 OH2 WAT S. 61 | 19 809 49 810 61 716 1 00 1 |
| MOTA | | 2.00 46.14 |
| ATOM | | 00 42.23 |
| ATOM | | |
| ATOM | 2000 | 47.925 33.253 61.470 1.00 34.93 8 |
| ATOM | | 32.500 36.000 41.000 1.00 35.33 g |
| | 2054 | 2/.245 56.551 44.579 1.00 34 19 9 |
| MOTA | 3054 OH2 WAT S 67 | 5.176 32.914 54.669 1.00 41.89 8 |
| ATOM | 3055 OH2 WAT S 68 | 41.159 51.018 49.348 1.00 27.31 8 |
| ATOM | 3056 OH2 WAT S 69 | 12 869 50 209 61 977 1 00 00 |
| ATOM | 3057 OH2 WAT S 70 | 17 499 12 926 67 074 |
| ATOM | 3058 OH2 WAT S 71 | 27 152 12 199 53 000 1 00 44.91 8 |
| MOTA | 3059 OH2 WAT S 72 | 25 213 54 909 67 900 1 00 10.70 8 |
| ATOM | 3060 OH2 WAT S 73 | 1,00 01.35 |
| ATOM | 3061 OH2 WAT S 74 | 22 765 |
| ATOM | 3062 CH2 WAT S 75 | 1.00 21.01 8 |
| ATOM | 3063 OH2 WAT S 76 | 35.535 27.040 70.698 1.00 34.04 8 |
| ATOM | 3064 OH2 WAT S 77 | 20.280 16.065 76.564 1.00 32.20 8 |
| ATOM | 2065 | 18.451 25.555 45.150 1.00 28.55 8 |
| ATOM | | 10.446 61.273 48.633 1.00 44.74 8 |
| | 2000 | 13.256 24.051 73.017 1.00 35.45 8 |
| ATOM | 3067 OH2 WAT S 80 | 23.571 13.292 69.937 1.00 49.49 8 |
| MOTA | 3068 OH2 WAT S 81 | 29.891 18.071 46.109 1.00 22.84 8 |
| MOTA | 3069 OH2 WAT S 82 | 12 886 49 773 75 009 3 00 |
| MOTA | 3070 OH2 WAT S 83 - | 41 349 15 471 45 004 + 00 |
| MOTA | 3071 OH2 WATS 84 | 13 406 44 647 71 240 |
| ATOM | 3072 OH2 WAT S 85 | 30 444 35 317 51 000 3 00 00 |
| ATOM | 3073 OH2 WAT S 86 | 5 217 40 817 53 244 2 20 30 13 8 |
| ATOM | 3074 CH2 WAT S 87 | 1.00 19.31 8 |
| ATOM | 3075 OH2 WAT S 88 | 1.00 30.72 8 |
| ATOM | 3076 OH2 WAT S 89 | 41.816 25.022 72.452 1.00 22.92 8 |
| ATOM | 3.000 | 50.621 36.644 60.248 1.00 29.29 8 |
| ATOM | 2000 | 26.008 34.532 49.627 1.00 45.42 8 |
| ATOM | 2004 | 8.131 39.168 54.903 1.00 31.50 8 |
| | | 16.591 58.091 57.551 1.00 34.73 8 |
| ATOM | 3080 OH2 WAT S 93 | 34.773 54.065 69.382 1.00 36.05 8 |
| MOTA | 3081 OH2 WAT 5 94 | 42.105 31.720 71.257 1.00 35.49 R |
| MOTA | 3082 OH2 WAT S 95 | 29.684 52.077 73.172 1.00 35.17 8 |
| atom | 3083 OH2 WAT S 96 | 26.411 37.426 38.934 1.00 41.68 8 |
| ATOM | 3084 OH2 WAT S 97 | 41 193 E2 000 C2 000 |
| ATOM | 3085 CH2 WAT S 98 | 21 165 |
| MOTA | 3086 OH2 WAT S 99 | 25 060 19 095 36 550 |
| MOTA | 3087 OH2 WAT S 100 | 37 304 30 032 73 700 1 00 70 8 |
| MOTA | 3088 OH2 WAT S 101 | 1.00 23.33 |
| MOTA | 3089 CH2 WAT S 102 | 1.00 29.00 8 |
| ATOM | 3090 OH2 WAT S 103 | 24 000 |
| MOTA | 3091 OH2 WAT S 104 | 24.029 42.997 74.111 1.00 25.23 8 |
| | 3092 OH2 WAT S 104 | 42.477 21.773 46.986 1.00 49.05 8 |
| ATOM | | 49.984 22.945 31.397 1 00 44 21 0 |
| MOTA | 3093 OH2 WAT S 106 | 40.850 36.936 31.885 1.00 43.26 g |
| MOTA | 3094 CH2 WAT S 107 | 9.750 32.487 48.823 1.00 35.71 8 |
| MOTA | 3095 OH2 WAT S 108 | 7.618 30.171 58.896 1.00 40.03 8 |
| MOTA | 3096 OH2 WAT 5 109 | 17 602 12 884 60 865 |
| MOTA | 3097 CH2 WAT S 110 | 22 590 0 244 67 504 |
| MOT | 3098 OH2 WAT S 111 | 21 034 20 704 06 064 1.00 33.01 8 |
| MOTA | 3099 OH2 WAT S 112 | 24.791 14.674 50.001 1.00 50.02 8 |
| TOM | 3100 OH2 WAT S 113 | 40 750 47 404 54 056 1 00 45 00 |
| MOT | 3101 OH2 WAT S 114 | 7 708 42 470 50 000 1.00 40.36 8 |
| MOT | 3102 OH2 WAT S 115 | 32 375 40 136 77 566 |
| | | 32.375 49.136 77.566 1.00 27.53 8 |
| | | |

| 3 TOM | 3103 | OH2 WAT 5 116 | 5.596 | 17.009 | 64.551 | 1.00 39.15 | 8 |
|-------|-------|---------------|----------|--------|--------|-------------|-----|
| ATOM | 3104 | OH2 WAT S 117 | | 50.998 | 70.563 | 1.00 19.73 | 8 |
| ATOM | | | | 64.927 | 64.164 | 1.00 27.16 | 8 |
| ATOM | 3105 | OH2 WAT S 118 | | 43.601 | 46.279 | 1.00 32.31 | 8 |
| ATOM | 3106 | OH2 WAT S 119 | | | | 1.00 55.20 | 8 |
| MOTA | 3107 | OH2 WAT S 120 | | 24.398 | 46.723 | | |
| MOTA | 3108 | OH2 WAT S 121 | | 16.122 | 54.229 | 1.00 35.91 | 8 |
| ATOM | 3109 | OH2 WAT S 122 | 26.772 | 34.085 | 33.852 | 1.00 37.49 | 8 |
| | 3110 | OH2 WAT S 123 | 28.654 | 37.783 | 75.829 | 1.00 47.30 | 8 |
| ATOM | | OH2 WAT S 124 | 49.180 | 22.653 | 59.678 | 1.00 37.33 | 8 |
| ATOM | 3111 | OHZ WAI 3 124 | | 27.788 | 65.975 | 1.00 67.86 | 8 |
| MOTA | 3112 | OH2 WAT S 125 | 20.301 | 13.344 | 57.366 | 1.00 36.18 | 8 |
| MOTA | 3113 | OH2 WAT S 126 | 34.251 | | | 1.00 33.63 | 8 |
| MOTA | 3114 | OH2 WAT S 127 | 49.215 | 36.854 | 48.117 | | |
| ATOM | 3115 | OH2 WAT S 128 | 45.826 | 19.588 | 41.601 | 1.00 44.07 | 8 |
| ATOM | .3116 | OH2 WAT S 129 | 18.693 | 56.382 | 64.014 | 1.00 47.77 | 8 |
| | 3117 | OH2 WAT S 130 | | 24.202 | 36.963 | 1.00 32.70 | 8 |
| MOTA | | OH2 WAT S 131 | | 51.901 | 38.133 | 1.00 54.07 | 8 |
| ATOM | 3118 | | | 36.558 | 48.679 | 1.00 42.21 | . 8 |
| ATOM | 3119 | OH2 WAT S 132 | | 26.029 | 34.353 | 1.00 56.33 | _ |
| MOTA | 3120 | OH2 WAT S 133 | 46.851 | | 68.647 | 1.00 45.99 | 8 |
| ATOM | 3121 | OH2 WAT S 134 | | 41.533 | | | |
| MOTA | 3122 | OH2 WAT S 135 | | 38.382 | 78.167 | 1.00 44.50 | 8 |
| ATOM | 3123 | OH2 WAT S 136 | 6.384 | 19.317 | 71.166 | 1.00 28.17 | 8 |
| ATOM | 3124 | OH2 WAT S 137 | 17.982 | 39.823 | 66.487 | 1.00 49.31 | 8 |
| | 3125 | OH2 WAT S 138 | | 22.286 | 61.863 | 1.00 43.42 | 8 |
| MOTA | 3126 | OH2 WAT S 139 | | 14.196 | 55.622 | 1.00 35.55 | 8 |
| ATOM | | | | 33.180 | 80.320 | 1.00 43.94 | 8 |
| MOTA | 3127 | | | 32.906 | 27.392 | 1.00 24.82 | 8 |
| MOTA | 3128 | OH2 WAT 5 141 | | | 64.002 | 1.00 41.93 | 8 |
| MOTA | 3129 | OH2 WAT S 142 | 33.971 | 3.859 | | 1.00 49.03 | 8 |
| ATOM | 3130 | OH2 WAT S 143 | 27.314 | 8.087 | 70.916 | | |
| MOTA | 3131 | OH2 WAT S 144 | 4.310 | 39.006 | 64.550 | 1.00 32.70 | 8 |
| ATOM | 3132 | OH2 WAT S 145 | 2.940 | 19.950 | 63.265 | 1.00 33.24 | 8 |
| | 3133 | OH2 WAT S 146 | | 47.625 | 60.121 | 1.00 44.24 | 8 |
| MOTA | | OH2 WAT S 147 | | 53.746 | 42.337 | 1.00 47.82 | 8 |
| MOTA | 3134 | OH2 WAT S 148 | 32.767 | 38.897 | 49.651 | 1.00 21.86 | 8 |
| MOTA | 3135 | | | 57.288 | 47.392 | 1.00 36.13 | 8 |
| MOTA | 3136 | OH2 WAT S 149 | | 18.011 | 32.273 | 1.00 38.04 | 8 |
| ATOM | 3137 | OH2 WAT S 150 | | | 55.583 | 1.00 41.68 | 8 |
| ATOM | 3138 | OH2 WAT S 151 | 24.054 | 43.182 | | 1.00 60.62 | 8 |
| ATOM | 3139 | OH2 WAT S 152 | 27.686 | 64.936 | 52.937 | | 8 |
| ATOM | 3140 | OH2 WAT S 153 | 24.084 | 39.543 | 76.589 | 1.00 22.62 | |
| MOTA | 3141 | OH2 WAT S 154 | 42.110 | 10.159 | 68.662 | 1.00 46.98 | 8 |
| | 3142 | OH2 WAT S 15 | 9.675 | 22.905 | 75.335 | 1.00 26.45 | 8 |
| MOTA | 3143 | OH2 WAT S 150 | | 34.799 | 52.857 | 1.00 33.84 | 8 |
| ATOM | | OH2 WAT S 15 | | 35.051 | 76.446 | 1.00 36.27 | 8, |
| ATOM | 3144 | | | 58.311 | 60.390 | 1.00 54.69 | 8 |
| MOTA | 3145 | | | 58.378 | 71.881 | 1.00 28.59 | 8 |
| MOTA | 3146 | OH2 WAT S 15 | | | 56.138 | 1.00 37.67 | 8 |
| ATOM | 3147 | OH2 WAT S 160 | 11.829 | 60.543 | 67.935 | 1.00 56.62 | 8 |
| ATOM | 3148 | OH2 WAT S 16 | 24.24 | 48.010 | | 1.00 29.88 | 8 |
| ATOM | 3149 | OH2 WAT S 163 | ز 12.85 | 33.929 | 77.503 | | |
| ATOM | 3150 | OH2 WAT S 163 | 9.49` | 26.168 | 59.687 | 1.00 15.42 | 8 |
| | 3151 | OH2 WAT S 164 | 27.424 | 16.480 | 38.895 | 1.00 36.86 | 8 |
| ATOM | 3152 | OH2 WAT S 16 | | 56.634 | 49.614 | 1.00 30.08 | 8 |
| ATOM | | OH2 WAT S 160 | | 13.394 | 57.919 | 1.00 39.47 | 8 |
| MOTA | 3153 | OH2 WAT 3 100 | | 38.223 | 73.903 | .1.00 29.50 | 8 |
| MOTĄ | 3154 | OH2 WAT S 16 | | 48.023 | 74.119 | 1.00 38.12 | 8 |
| MOTA | 3155 | OH2 WAT S 16 | | | 33.116 | 1.00 24.47 | 8 |
| ATOM | 3156 | OH2 WAT 5 169 | 42.092 | 39.503 | | 1.00 38.65 | 8 |
| ATOM | 3157 | OH2 WAT S 17 | 34.547 | 12.749 | 38.054 | 1.00 30.03 | |
| ATOM | 3158 | OH2 WAT S 17 | 15.377 | 60.862 | 50.791 | 1.00 32.82 | 8 |
| | 3159 | OH2 WAT S 17 | 31.854 | 42.110 | 62.950 | 1.00 42.43 | 8 |
| MOTA | | OH2 WAT S 17 | | 44.073 | 57.626 | 1.00 34.04 | 8 |
| ATOM | 3160 | OH2 WAT S 17 | | 50.038 | 42.232 | 1.00 32.87 | 8 |
| Mota | 3161 | ONZ WAT 5 17 | | 18.280 | 53.455 | 1.00 40.51 | 8 |
| ATOM | 3162 | OH2 WAT S 17 | | 37.509 | 53.943 | 1.00 40.43 | 8 |
| ATOM | 3163 | OH2 WAT S 17 | | | 70.642 | 1.00 47.97 | 8 |
| ATOM | 3164 | OH2 WAT S 17 | 23.921 | 47.029 | | 1.00 62.12 | 8 |
| MOTA | 3165 | OH2 WAT S 178 | 3 27.974 | 47.778 | 69.949 | 1.00 62.12 | |
| ATOM | 3166 | OH2 WAT 5 17 | 7.850 | 25.093 | 51.345 | 1.00 50.13 | 8 |
| | 3167 | OH2 WAT S 18 | 22.080 | 48.840 | 66.463 | 1.00 53.81 | 8 |
| MOTA | | OH2 WAT S 18 | | 48.220 | 77.419 | 1.00 30.86 | 8 |
| MOTA | 3168 | UNZ WAI 5 10 | | | - | • | |
| | | • | | | | | |

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Figure 17-49

| | MOTA | 3169 | OH2 WAT S | 182 | 43.893 | . 35.526 | 52.018 | 1.00 47.14 | 8 |
|---|-------|------|-------------|---------|--------|----------|--------|------------|-----|
| | ATOM | 3170 | | 183 | 29.166 | 21.424 | 28.950 | 1.00 45.08 | 8 |
| | MOTA | 3171 | OH2 WAT S | 184 | 51.175 | 51.545 | 62.599 | 1.00 33.88 | 8 |
| | ATOM | 3172 | OH2 WAT S | 185 | 18.520 | 46.208 | 42.323 | 1.00 50.85 | 8 |
| | MOTA | 3173 | OH2 WAT S | | 44.774 | 30.219 | 38.653 | 1.00 45.36 | 8 |
| | MOTA | 3174 | OH2 WAT S | 187 : | 30.770 | 9.460 | 69.837 | 1.00 32.44 | 8 |
| | MOTA | 3175 | OH2 WAT S | 188 | 22.157 | 39.535 | 78.736 | 1.00 37.01 | 8 |
| | MOTA | 3176 | OH2 WAT S | 189 | 11.778 | 50.526 | 68.987 | 1.00 41.34 | 8 |
| | MOTA | 3177 | OH2 WAT S | 190 | 31.339 | 60.910 | 49.439 | 1.00 21.88 | 8 |
| | MOTA | 3178 | OH2 WAT S | 191 3 | 31.165 | 14.244 | 74.907 | 1.00 27.47 | 8 |
| | ATOM | 3179 | OH2 WAT S | | 39.705 | 15.398 | 70.464 | 1.00 47.05 | 8 |
| | ATOM | 3180 | OH2 WAT S | 193 | 3.668 | 34.304 | 72.937 | 1.00 39.82 | 8 |
| | ATOM- | 3181 | OH2 WAT S | 194 2 | 25.256 | 9.360 | 67.925 | 1.00 33.21 | 8 |
| | ATOM | 3182 | OH2 WAT S | | 17.575 | 17.667 | 48.773 | 1.00 40.79 | 8 |
| | ATOM | 3183 | OH2 WAT S | 196 3 | 2.017 | 13.045 | 34.633 | 1.00 37.00 | . 8 |
| | MOTA | 3184 | OH2 WAT S | 197 3 | 5.476 | 7.006 | 64.436 | 1.00 49.59 | , 8 |
| | MOTA | 3185 | OH2 WAT S | 198 1 | 2.180 | 16.270 | 56.288 | 1.00 47.22 | 8 |
| | MOTA | 3186 | OH2 WAT S | 199 🧎 3 | 7.133 | 21.226 | 75.963 | 1.00 38.59 | 8 |
| | ATOM | 3187 | OH2 WAT S | 200 4 | 0.268 | 15.712 | 48.199 | 1.00 39.24 | 8 |
| • | MOTA | 3188 | OH2 WAT S | 201 2 | 5.159 | 17.768 | 46.858 | 1.00 49.88 | 8 |
| | ATOM | 3189 | OH2 WAT S | | 4.593 | 27.104 | 65.727 | 1.00 53.46 | 8 |
| | MOTA | 3190 | OH2 WAT S 2 | 203 3 | 6.741 | 20.267 | 33.858 | 1.00 41.90 | 8 |
| | MOTA | 3191 | | 204 1 | 0.013 | 53.930 | 47.546 | 1.00 48.06 | 8 |
| | ATOM | 3192 | | | 2.305 | 16.731 | 54.471 | 1.00 27.07 | 8 |
| | MOTA | 3193 | | | 7.454 | 34.778 | 74.101 | 1.00 47.44 | 8 |
| | ATOM | 3194 | OH2 WAT S 2 | | 5.189 | 55.767 | 45.193 | 1.00 59.49 | 8 |
| | ATOM | 3195 | | | 7.827 | 18.151 | 36.382 | 1.00 45.31 | 8 |
| | ATOM | 3196 | | | 6.823 | 37.405 | 51.989 | 1.00 58.23 | 8 |
| | ATOM | 3197 | | | 2.040 | 43.551 | 36.157 | 1.00 30.78 | 8 |
| | MOTA | 3198 | | | 7.038 | 52.360 | 63.283 | 1.00 34.08 | 8 |
| | ATOM | 3199 | | | 0.001 | 18.471 | 49.568 | 1.00 33.92 | 8 |
| | MOTA | 3200 | | | 3.045 | 28.615 | 33.729 | 1.00 44.22 | 8 |
| | ATOM | 3201 | | | 6.130 | 61.496 | 75.246 | 1.00 40.49 | 8 |
| | MOTA | 3202 | | | 3.881 | 32.473 | 46.604 | 1.00 39.35 | 8 |
| | ATOM | 3203 | OH2 WAT S 2 | | | 45.987 | 44.362 | 1.00 36.50 | 8 |
| | ATOM | 3204 | OH2 WAT S 2 | | 6.925 | 42.281 | 65.917 | 1.00 34.22 | 8 |
| | MOTA | 3205 | OH2 WAT S 2 | 18 32 | 2.823 | 8.977 | 59.213 | 1.00 27.03 | 8 |
| | END | | | | | | | | |

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| Figure 18-1 | | | | | | | | | |
|--------------|----------|-----------|-------|----------|------------------|------------------|--------------------|--------------------------|----|
| | | | | Residue | e # X | Y | Z 138.208 | B Segment 1.00 56.80 | ŤΩ |
| MOTA | 1 | CB | ALA A | _ | 46.726 47.943 | 14.971 12.813 | 138.561 | 1.00 58.93 | |
| ATOM | 2 3 | 0 | ALA A | _ | 48.857 | 13.292 | 137.884 | 1.00 60.99 | |
| ATOM ATOM | 4 | N | ALA A | _ | 46.995 | 14.046 | 140.488 | 1.00 56.88 | |
| ATOM | 5 | CA | ALA A | _ | 46.801 | 13.697 | 139.052 | 1.00 59.41 | |
| ATOM- | 6 | N | LYS A | . 3 | 47.890 | 11.525 | 138.903 | 1.00 53.81 | |
| MOTA | 7 | CA | LA2 y | _ | 48.937 | 10.591 | 138.492 | 1.00 53.62 1.00 50.26 | |
| MOTA | 8 | CB | LYS A | | 48.736 48.917 | 9.229 9.279 | 139.156 140.665 | 1.00 56.64 | |
| MOTA | 9 | CG | LYS A | | 48.950 | 7.891 | | 1.00 57.18 | |
| MOTA | 10 11 | CE | LYS A | _ | 49.160 | 7.964 | | 1.00 56.74 | |
| ATOM ATOM | 12 | NZ | LYS A | _ | 50.423 | | 143.165 | 1.00 54.86 | |
| ATOM | 13 | C | LYS A | _ | 49.063 | | 136.986 | 1.00 49.95 | |
| MOTA | 14 | 0 | LYS A | | 48.088 | 10.562 | 136.248 136.550 | 1.00 44.34 1.00 46.01 | |
| MOTA | 15 | N | VALA | _ | 50.287 50.609 | 10.147 9.985 | 135.142 | 1.00 42.48 | |
| ATOM | 16 | CA | VAL A | | 51.901 | 10.755 | 134.809 | 1.00 43.42 | |
| ATOM | 17 18 | CB | VAL A | | 52.179 | 10.713 | 133.307 | 1.00 39.20 | |
| ATOM ATOM | 19 | | VAL A | | 51.773 | 12.186 | 135.310 | 1.00 39.34 | |
| ATOM | 20 | C | VAL A | 4 | 50.787 | | 134.806 | 1.00 38.41 1.00 37.08 | |
| MOTA | 21 | 0 | VAL | | 51.659 | 8.011 | 135.351 133.899 | 1.00 37.08 | |
| MOTA | 22. | N | LYS A | | 49.959 50.016 | 6.610 | 133.515 | 1.00 38.17 | |
| ATOM | 23 24 | CA CB | LYS A | | 48.700 | 5.915 | 133.887 | 1.00 38.40 | |
| ATOM ATOM | 25 | CG | LYS A | •_ | 48.411 | 5.803 | 135.385 | 1.00 42.84 | |
| ATOM | 26 | CD | LYS A | 5 | 49.384 | 4.855 | 136.070 | 1.00 44.10 | |
| MOTA | 27 | CE | LYS A | | 49.017 | 4.632 | 137.534 138.322 | 1.00 45.97 1.00 51.78 | |
| ATOM | 28 | NZ | LYS A | | 49.045 50.275 | 5.894 6.392 | 132.030 | 1.00 38.31 | |
| ATOM | 29 | С | LYS A | _ | 49.992 | 7.253 | 131.201 | 1.00 38.13 | |
| MOTA MOTA | 30 31 | N O | LEU 3 | _ | 50.817 | 5.220 | 131.717 | 1.00 35.05 | |
| ATOM | 32 | CA | LEU A | - | 51.082 | 4.818 | | 1.00 31.46 | |
| ATOM | 33 | CB | LEU A | | 52.582 | 4.592 | | 1.00 28.46 1.00 30.91 | |
| ATOM | 34 | CG | LEU A | | 53.094 52.618 | 4.256 2.884 | | 1.00 33.05 | |
| ATOM | 35 | | LEU A | | 52.630 | 5.312 | | 1.00 21.96 | |
| atom atom | 36 37 | CDZ | LEU A | | 50.307 | 3.512 | 130.164 | 1.00 30.50 | |
| ATOM | 38 | ō | LEU Z | _ | 50.453 | 2.581 | | 1.00 32.82 | |
| ATOM | 39 | N | ILE A | | 49.459 | 3.456 | | 1.00 26.94 1.00 28.29 | |
| MOTA | 40 | CA | ILE A | | 48.676 47.218 | 2.255 | 128.493 | 1.00 28.94 | |
| ATOM | 41 42 | CB | ILE A | | 46.499 | 1.343 | | 1.00 32.57 | |
| MOTA MOTA | 43 | CG1 | | | 46.447 | 3.172 | 129.688 | 1.00 36.59 | |
| ATOM | 44 | | ILE | _ | 46.979 | 4.468 | 130.236 | 1.00 46.80 | |
| MOTA | 45 | С | ILE | | 49.341 | 1.470 | | 1.00 31.09 1.00 27.65 | |
| ATOM | 46 | 0 | IL- | a 7 | 49.600 | 2.009 0.201 | | 1.00 27.30 | |
| ATOM | 47 | N | ·GL. | | 49.638 50.277 | -0.614 | | 1.00 25.50 | |
| MOTA | 48 49 | CA C | GLY A | | 50.578 | -2.024 | 127.480 | 1.00 30.66 | |
| ATOM ATOM | 50 | ŏ | GLY | | 50.224 | -2.421 | 128.592 | 1.00 30.02 | |
| ATOM | 51 | N | THR . | A 9 | 51.238 | -2.777 | 126.611 | 1.00 28.94 1.00 33.63 | |
| MOTA | 52 | CA | THE. | | 51.614 | -4.156 | 126.877 126.857 | 1.00 36.19 | |
| MOTA | 53 | CB | THR . | | 50.393 50.827 | -6.441 | | 1.00 34.87 | |
| ATOM | 54 55 | OG1 | THR . | | 49.633 | -4.931 | 125.548 | 1.00 36.49 | |
| MOTA MOTA | 56 | C | THR | | 52.567 | -4.637 | 125.794 | 1.00 34.83 | |
| MOTA | 57 | ō | THR | A 9 | 52.545 | -4.133 | | 1.00 36.91 1.00 39.15 | |
| ATOM | 58 | N | LEU . | A 10 | 53.407 | -5.609 | | 1.00 39.15 | |
| atom | 59 | CA | LEU | | 54.345 55.402 | -6.167 -7.009 | | 1.00 42.40 | |
| MOTA | 60 | CB | LEU | | 56.482 | -6.282 | 126.687 | 1.00 42.29 | |
| ATOM | 61 62 | CG CD1 | LEU | A 10 | 55.870 | -5.293 | 3 127.647 | 1.00 42.92 | |
| atom atom | 63 | | LEU | | 57.319 | -7.306 | 127.424 | 1.00 40.29 | |
| ATOM | 64 | c | LEU | A 10 | 53.591 | -7.039 | 124.159 | 1.00 41.70 | |
| ATOM | 65 | 0 | LEU | | 54.055 | -7.266 | 123.044 124.557 | 1.00 37.13 | |
| MOTA | 66 | N | ASP | A 11 | 52.419 | -/.512 | ,, | | |
| | | | | | | | | | |

| MOTA | 67 CA ASP A 11 | 51.617 -8.369 123.683 1.00 53.30 |
|--------------|------------------------------------|--|
| MOTA | 68 CB ASP A 11 | 50.230 -8.608 124.287 1.00 52.35 |
| ATOM | 69 .CG ASP A 11 | 50.295 -9.331 125.610 1.00 53.33 |
| ATOM | 70 OD1 ASP A 11 | 51.004 -10.358 125.685 1.00 52.21 |
| ATOM | 71 OD2 ASP A 11 | 49.630 -8.883 126.567 1.00 58.48 |
| MOTA | 72 C ASP A 11 | 51.459 -7.840 122.257 1.00 53.33 |
| ATOM | 73 O ASP A 11 | 51.360 -8.626 121.311 1.00 54.31 |
| MOTA | 74 N TYR A 12 | 51.424 -6.521 122.092 1.00 51.92 |
| MOTA | 75 CA TYR A 12 | 51.275 -5.970 120.749 1.00 51.41 |
| MOTA | 76 CB TYR A 12 | 51.328 -4.437 120.755 1.00 49.05 |
| ATOM | 77 CG TYR A 12 | 50.164 -3.729 121.421 1.00 45.48 |
| ATOM | 78 CD1 TYR A 12 | 50.296 -3.157 122.686 1.00 47.08 |
| ATOM | 79 CE1 TYR A 12 | 49.252 -2.430 123.263 1.00 47.53 |
| ATOM | 80 CD2 TYR A 12 | 48.952 -3.565 120.749 1.00 43.77 |
| ATOM | 81 CE2 TYR A 12 | 47.906 ~2.847 121.310 1.00 44.16 |
| ATOM | 82 CZ TYR A 12 | 48.061 -2.279 122.566 1.00 48.67 |
| MOTA | 83 OH TYR A 12 | 47.030 -1.548 123.116 1.00 48.65 |
| ATOM | 84 C TYR A 12 | 52.367 -6.503 119.816 1.00 50.01 |
| ATOM | 85 O TYR A 12 | 52.197 -6.525 118.596 1.00 45.56 |
| ATOM | 86 N GLYA 13 | 53.484 -6.931 120.396 1.00 48.72 |
| MOTA | 87 CA GLY A 13 | 54.574 -7.458 119.599 1.00 50.56 |
| MOTA | 88 C GLY A 13 | 54.196 -8.727 118.857 1.00 53.32 |
| ATOM | 89 O GLY A 13 | 54.931 -9.184 117.982 1.00 52.64 |
| MOTA | 90 N LYS A 14 | 53.045 -9.294 119.207 1.00 53.37 |
| MOTA | 91 CA LYS A 14 | 52.555 -10.518 118.579 1.00 54.56 |
| ATOM | 92 CB LYS A 14 | 52.022 -11.475 119.653 1.00 58.02 |
| MOTA | 93 CG LYS A 14 | 53.086 -12.062 120.591 1.00 62.81 |
| ATOM | 94 CD LYS A 14 | 53.934 -13.154 119.918 1.00 61.61 |
| MOTA | 95 CE LYS A 14 | 54.747 -12.638 118.734 1.00 61.77 |
| ATOM | 96 NZ LYS A 14 | 55.514 -13.713 118.045 1.00 58.35 |
| MOTA | 97 C LYS A 14 | 51.455 -10.231 117.559 1.00 52.03 |
| ATOM ATOM | 98 O LYS A 14 99 N TYR A 15 | 50.911 -11.145 116.942 1.00 51.71 |
| ATOM | | 51.143 -8.955.117.372 1.00 46.92 |
| ATOM | | 50.091 -8.563 116.449 1.00 47.99 |
| ATOM | 101 CB TYR A 15 102 CG TYR A 15 | 48.959 -7.915 117.253 1.00 50.40 |
| ATOM | 103 CD1 TYR A 15 | 48.456 -8.793 118.386 1.00 53.01 48.166 -8.255 119.637 1.00 52.10 |
| ATOM | 104 CE1 TYR A 15 | |
| ATOM | 105 CD2 TYR A 15 | ** *** |
| ATOM | 106 CE2 TYR A 15 | 48.283 -10.166 118.208 1.00 54.67 47.838 -10.976 119.250 1.00 55.69 |
| ATOM | 107 CZ TYR A 15 | 47.561 -10.412 120.485 1.00 54.18 |
| MOTA | 108 OH TYR A 15 | 47.130 -11.208 121.520 1.00 55.42 |
| ATOM | 109 C TYR A 15 | 50.592 -7.617 115.353 1.00 46.20 |
| MOTA | 110 O TYR A 15 | 49.933 -6.635 115.018 1.00 43.72 |
| ATOM | 111 N ARG A 16 | 51.758 -7.924 114.791 1.00 46.29 |
| MOTA | 112 CA ARG A 16 | 52.347 -7.109 113.727 1.00 45.66 |
| ATOM | 113 CB ARG A 16 | 53.779 -7.545 113.441 1.00 50.56 |
| ATOM | 114 CG ARG A 16 | 54.677 -7.698 114.636 1.00 56.90 |
| ATOM | 115 CD ARG A 16 | 54.992 -6.388 115.315 1.00 60.72 |
| MOTA | 116 NE ARG A 16 | 56.021 -6.602 116.328 1.00 66.70 |
| MOTA | 117 CZ ARG A 16 | 57.211 -7.141 116.070 1.00 66.68 |
| MOTA | 118 NH1 ARG A 16 | 57.520 -7.519 114.834 1.00 65.68 |
| ATOM | 119 NH2 ARG A 16 | 58.093 -7.314 117.046 1.00 66.33 |
| MOTA | 120 C ARG A 16 | 51.573 -7.298 112.429 1.00 44.20 |
| ATOM NOW | 121 O ARG A 16 122 N TYR A 17 | 50.871 -8.293 112.254 1.00 43.41 |
| atom Atom | | 51.715 -6.346 111.514 1.00 39.23 |
| ATOM | 123 CA TYR A 17 124 CB TYR A 17 | 51.067 -6.453 110.215 1.00 38.71 50.913 -5.072 109.565 1.00 33.83 |
| ATOM . | 124 CS 11R A 17 | |
| ATOM | 126 CD1 TYR A 17 | |
| ATON | 127 CE1 TYR A 17 | |
| ATOM | 128 CD2 TYR A 17 | |
| ATOM | 129 CE2 TYR A 17 | 48 888 |
| TOM | 130 CZ TYR A 17 | 47.752 -2.925 109.656 1.00 26.34 47.626 -2.659 111.009 1.00 27.28 |
| ATCM | 131 OH TYR A 17 | 46.602 -1.842 111.450 1.00 22.04 |
| ATOM | 132 C TYR A 17 | 51.972 -7.350 109.368 1.00 41.52 |
| | | |

Figure 18-3

| | | _ | - | | | 4 | 0 505 | 100 600 | |
|--------|-------|-----|---------|-----|-------|--------|---------|---------|------------|
| ATOM | 133 | 0 | TYR A | 17 | | 53.150 | | 109.683 | 1.00 35.63 |
| MOTA | 134 | N | PRO A | 18 | | 51.440 | -7.925 | 108.278 | 1.00 46.68 |
| MOTA | 135 | CD | PRO A | 18 | | 50.076 | -7.765 | 107.755 | 1.00 47.16 |
| | 136 | CA | PRO A | | | 52.205 | -8.812 | | 1.00 48.87 |
| ATOM | | | | 18 | | | | | |
| ATOM | 137 | CB | PRO A | 18 | | 51.213 | -9.091 | | 1.00 48.14 |
| ATOM | 138 | CG | PRO A | 18 | | 50.343 | -7.837 | 106.274 | 1.00 55.13 |
| MOTA | 139 | С | PRO A | 18 | | 53.556 | -8.303 | 106.885 | 1.00 49.67 |
| | 140 | | | | | | | 106.766 | 1.00 49.33 |
| ATOM | | 0 | PRO A | 18 | | 53.788 | | | |
| MOTA | 141 | N | LYS A | 19 | | 54.432 | -9.261 | | 1.00 53.22 |
| ATOM | 142 | CA | LYS A | 19 | | 55.800 | -9.044 | 106.114 | 1.00 57.00 |
| ATOM | 143 | CB | LYS A | 19 | | | -10.242 | | 1.00 62.34 |
| | | | | | | | | | |
| ATOM | 144 | CG | LYS A | 19 | | 55.069 | | | 1.00 67.94 |
| ATOM | 145 | CD | LYS A | 19 | | 54.239 | -9.963 | | 1.00 70.76 |
| ATOM | 146 | CE | LYS A | 19 | | 53.004 | -10.653 | 103.162 | 1.00 73.70 |
| ATOM | 147 | NZ | LYS A | 19 | | 52.116 | -9.701 | | 1.00 79.01 |
| | | | | | | 56.229 | -7.757 | | 1.00 55.93 |
| MOTA | 148 | С | LYS A | 19 | | | | | |
| MOTA | 149 | 0 | LYS A | 19 | | 57.230 | -7.150 | | 1.00 59.86 |
| ATOM | 150 | N | ASN A | 20 | | 55.515 | -7.338 | 104.367 | 1.00 49.62 |
| MOTA | 151 | CA | ASN A | 20 | | 55.925 | -6.130 | 103.652 | 1.00 50.02 |
| | | | | | | 55.829 | -6.359 | | 1.00 50.62 |
| ATOM | 152 | CB | ASN A | 20 | | | | | |
| ATOM | 153 | CG | ASN A | 20 | | 56.729 | -7.487 | | 1.00 51.26 |
| MOTA | 154 | OD1 | . ASN A | 20 | | 57.948 | -7.437 | 101.843 | 1.00 46.88 |
| ATOM | 155 | ND2 | | 20 | | 56.130 | -8.513 | 101.074 | 1.00 50.85 |
| | | | | | | | | 104.023 | 1.00 45.50 |
| ATOM | 156 | С | ASN A | 20 | | 55.167 | -4.862 | | |
| ATOM | 157 | 0 | ASN A | 20 | | 55.481 | -3.778 | 103.533 | 1.00 45.35 |
| ATOM | 158 | N | HIS A | 21 | | 54.182 | -4.997 | 104.899 | 1.00 37.46 |
| ATOM | 159 | CA | HIS A | 21 | | 53.374 | -3.863 | 105.321 | 1.00 32.39 |
| | | CB | | 21 | | 52.198 | -4.355 | 106.162 | 1.00 29.34 |
| ATOM | 160 | | HIS A | | | | | | |
| ATOM | 161 | CG | HIS A | 21 | | 51.118 | -3.339 | 106.348 | 1.00 30.50 |
| ATOM | 162 | CD2 | HIS A | 21 | | 50.999 | -2.314 | 107.223 | 1.00 22.88 |
| ATOM | 163 | ND1 | HIS A | 21 | | 49.993 | -3.298 | 105.552 | 1.00 30.15 |
| | | | HIS A | 21 | | 49.226 | -2.293 | 105.933 | 1.00 30.96 |
| ATOM | 164 | | | | | | | | |
| ATOM | 165 | NE2 | | 21 | | 49.814 | -1.680 | 106.945 | 1.00 36.41 |
| ATOM | 166 | C | HIS A | 21 | | 54.194 | -2:879 | 106.155 | 1.00 29.18 |
| ATOM | 167 | 0 | HIS A | 21 | | 55.030 | -3.279 | 106.963 | 1.00 26.92 |
| | 168 | N | PRO A | 22 | | 53,965 | -1.572 | 105.969 | 1.00 31.12 |
| ATOM | | | | | | | | | 1.00 29.46 |
| ATOM | 169 | CD | PRO A | 22 | | 53.027 | -0.912 | 105.043 | |
| ATOM | 170 | CA | PRO A | 22 | | 54.702 | -0.567 | 106.739 | 1.00 29.27 |
| ATOM | 171 | CB | PRO A | 22 | : | 54.012 | 0.732 | 106.326 | 1.00 26.00 |
| ATOM | 172 | CG | PRO A | 22 | į | 53.670 | 0.434 | 104.875 | 1.00 31.52 |
| | | c | PRO A | | | 54.624 | -0.822 | 108.253 | 1.00 29.96 |
| ATOM | 173 | | | 22 | | | | | |
| ATOM | 174 | 0 | PRO A | 22 | | 55.575 | -0.538 | 108.981 | 1.00 27.47 |
| ATOM | 175 | N | LEU A | 23 | | 53.501 | -1.371 | 108.715 | 1.00 26.64 |
| MOTA | 176 | CA | LEU A | 23 | 9 | 53.309 | -1.644 | 110.144 | 1.00 30.44 |
| | 177 | СВ | LEU A | 23 | | 51.833 | -1.428 | 110.515 | 1.00 24.09 |
| MOTA | | | | | | | | | |
| MOTA | 178 | CG | LEU A | 23 | | 51.356 | 0.029 | 110.479 | 1.00 25.30 |
| ATCM | 179 | CD1 | LEU A | 23 | • • 4 | 19.836 | 0.103 | 110.668 | 1.00 17.72 |
| ATOM | 180 | CD2 | LEU A | 23 | 9 | 52.086 | 0.816 | 111.574 | 1.00 24.15 |
| ATOM | 181 | C | LEU A | 23 | | 3.775 | -3.015 | 110.662 | 1.00 31.64 |
| | | | | | | | -3.512 | 111.667 | 1.00 31.00 |
| ATCM | 182 | 0 | LEU A | 23 | | 3.252 | | | |
| ATOM | 183 | N | LYS A | 24 | | 4.753 | -3.636 | 110.012 | 1.00 28.25 |
| ATOM | 184 | CA | LYS A | 24 | 5 | 55.200 | ~4.929 | 110.513 | 1.00 30.90 |
| ATOM | 185 | CB | LYS A | 24 | | 55.718 | -5.810 | 109.372 | 1.00 36.59 |
| | | | LYS A | 24 | | 7.178 | -5.650 | 108.982 | 1.00 40.77 |
| atom | 186 | CG | | | | | | | |
| MOTA | 187 | CD | LYS A | 24 | | 7.546 | -4.259 | 108.535 | 1.00 44.61 |
| ATOM | 188 | CE | LYS A | 24 | | 8.858 | ~4.303 | 107.755 | 1.00 50.44 |
| ATOM | 189 | NZ | LYS A | 24 | | 9.959 | -4.990 | 108.487 | 1.00 51.30 |
| | | | | | | 6.282 | -4.736 | 111.581 | 1.00 32.57 |
| ATOM | 190 | С | LYS A | 24 | | | | | |
| MOTA | 191 | 0 | LYS A | 24 | | 6.695 | -5.683 | 112.245 | 1.00 29.83 |
| ATOM | 192 | N | ILE A | 25 | 5 | 6.729 | -3.497 | 111.750 | 1.00 27.06 |
| ATOM | 193 | CA | ILE A | 25 | | 7.755 | -3.200 | 112.739 | 1.00 30.45 |
| | 194 | | ILE A | 25 | | 8.416 | -1.822 | 112.499 | 1.00 33.37 |
| ATOM | | CB | | | | | | 111.120 | |
| ATOM | 195 | CG2 | ILE A | 25 | | 9.056 | -1.757 | | 1.00 33.22 |
| ATOM · | 196 | CG1 | ILE A | 25 | | 7.361 | -0.722 | 112.662 | 1.00 30.45 |
| ATCM | - 197 | CD1 | ILE A | 25 | 5 | 7.930 | 0.689 | 112.700 | 1.00 33.12 |
| | | CDI | ILE A | 25 | | 7.156 | -3.129 | 114.141 | 1.00 32.10 |
| ATCM | 198 | _ | | د ب | = | | -3.123 | | |

Figure 18-4

| ATOM | 199 O ILE A 25 | 55.967 -2.851 114.310 1.00 28.3 | ٦. |
|--------------|---------------------------------------|--|-----|
| ATOM | 200 N PRO A 26 | 57.979 -3.382 115.168 1.00 31.0 | |
| MOTA | 201 CD PRO A 26 | 59.395 -3.768 115.139 1.00 31.1 | |
| ATOM | 202 CA PRO A 26 | 57.507 -3.322 116.556 1.00 31.0 | |
| MOTA | 203 CB PRO A 26 | 58.709 -3.840 117.347 1.00 32.4 | |
| MOTA | 204 CG PRO A 26 | 59.454 -4.691 116.324 1.00 39.3 | |
| MOTA | 205 C PRO A 26 | 57.265 -1.840 116.827 1.00 28.4 | |
| ATOM | 206 O PRO A 26 | 58.001 -0.994 116.315 1.00 22.2 | 23 |
| MOTA MOTA | 207 N ARGA 27 208 CA ARGA 27 | 56.251 -1.514 117.614 1.00 24.1 | L6 |
| ATOM | 208 CA ARG A 27 209 CB ARG A 27 . | 55.977 -0.116 117.899 1.00 28.5 | |
| ATOM | 210 CG ARG A 27 | - 54.787 0.358 117.048 1.00 29.7 55.075 0.191 115.554 1.00 29.6 | |
| MOTA | 211 CD ARG A 27 | | 54 |
| ATOM | 212 NE ARG A 27 | 57 600 | |
| ATOM | 213 CZ ARG A 27 | 53.622 1.965 114.517 1.00 28.5 52.649 2.591 115.173 1.00 29.7 | |
| ATOM | 214 NH1 ARG A 27 | 51.857 1.924 115.999 1.00 30.1 | 7 |
| MOTA | 215 NH2 ARG A 27 | 52.451 3.889 114.983 1.00 23.2 | . , |
| MOTA | 216 C ARG A 27 | 55.746 0.114 119.387 1.00 30.7 | 11 |
| MOTA | 217 O ARG A 27 | 56.679 0.490 120.113 1.00 24.6 | |
| ATOM | 218 N VAL A 28 | 54.529 -0.117 119.863 1.00 23.5 | |
| ATOM | 219 CA VAL A 28 | 54.282 0.093 121.282 1.00 29.3 | |
| MOTA MOTA | 220 CB VAL A 28 221 CG1 VAL A 28 | 52.800 -0.124 121.635 1.00 34.5 | 6 |
| ATOM | 221 CG1 VAL A 28 222 CG2 VAL A 28 | 52.599 0.002 123.142 1.00 32.4 | 2 |
| ATOM | 223 C VAL A 28 | 51.947 0.908 120.903 1.00 33.7 55.158 -0.816 122.145 1.00 29.7 | 7 |
| ATOM | 224 O VAL A 28 | FF (77) | |
| ATOM | 225 N SER A 29 | FC 344 A 555 | |
| MOTA | 226 CA SER A 29 | 55.341 -2.059 121.718 1.00 26.0 56.162 -2.982 122.483 1.00 31.3 | פ |
| MOTA | 227 CB SER A 29 | 56.058 -4.399 121.905 1.00 26.9 | 2 |
| MOTA | 228 OG SER A 29 | 56.562 -4.464 120.579 1.00 33.8 | 5 |
| ATOM | 229 C SER A 29 | 57.609 -2.482 122.453 1.00 34.7 | |
| ATOM ATOM | 230 O SER A 29 231 N LEU A 30 | 58.378 -2.718 123.391 1.00 29.39 | 9 |
| ATOM | 231 N LEUA 30 232 CA LEUA 30 | 57.967 -1.778 121.380 1.00 31.20 | |
| ATOM | 233 CB LEU A 30 | 59.317 -1:234 121.240 1.00 32.00 59.554 -0.668 119.829 1.00 30.86 | |
| ATOM | 234 CG LEU A 30 | 61 000 | |
| ATOM | 235 CD1 LEU A 30 | 61.008 -0.550 119.333 1.00 33.22 61.066 0.484 118.224 1.00 28.76 | |
| ATOM | 236 CD2 LEU A 30 | 61.948 -0.135 120.441 1.00 35.11 | |
| MOTA | 237 C LEU A 30 | 59.423 -0.089 122.236 1.00 30.29 | |
| ATOM | 238 O LEU A 30 | 60.397 0.019 122.984 1.00 27.69 | |
| MOTA | 239 N LEU A 31 | 58.408 0.769 122.232 1.00 27.38 | 3 |
| ATOM ATOM | 240 CA LEU A 31 241 CB LEU A 31 | 58.372 1.915 123.126 1.00 24.94 | |
| ATOM | 241 CB LEU A 31 242 CG LEU A 31 | 57.008 2.596 123.042 1.00 24.92 | |
| ATOM | 243 CD1 LEU A 31 | 56.918 4.069 123.460 1.00 30.49 55.492 4.390 123.881 1.00 24.71 | |
| ATOM | 244 CD2 LEU A 31 | 55.492 4.390 123.881 1.00 24.71 57.851 4.355 124.603 1.00 27.32 | |
| ATOM | 245 C LEU A 31 | 58.610 1.429 124.564 1.00 28.18 | |
| ATOM | 246 O LEUA 31 | 59.489 1.928 125.263 1.00 33.64 | |
| MOTA | 247 N LEU A 32 | 57.831 0.445 125.000 1.00 30.17 | |
| ATOM | 248 CA LEU A 32 | 57.965 -0.084 126.357 1.00 30.59 | |
| MOTA | 249 CB LEU A 32 | 56.944 -1.206 126.601 1.00 30.55 | j |
| ATOM | 250 CG LEU A 32 | 55.458 -0.879 126.402 1.00 29.50 | |
| MOTA MOTA | 251 CD1 LEU A 32 .252 CD2 LEU A 32 | 54.611 -2.107 126.727 1.00 28.31 | |
| ATOM | 253 C LEU A 32 | 55.058 0.273 127.287 1.00 31.92 59.376 -0.597 126.657 1.00 33.56 | |
| ATOM | 254 O LEU A 32 | 50 061 | |
| ATOM | 255 N ARG A 33 | 59.961 -0.243 127.682 1.00 36.51 59.926 -1.429 125.777 1.00 29.75 | |
| ATOM | 256 CA ARG A 33 | 61.271 -1.953 125.999 1.00 33.49 | |
| ATOM | 257 CB ARG A 33 | 61.630 -3.003 124.945 1.00 39.50 | |
| ATOM | 258 CG ARG A 33 | 60.814 -4.283 125.024 1.00 44.40 | |
| MOTA | 259 CD ARG A 33 | 61.237 -5.256 123.933 1.00 53.68 | |
| MOTA | 260 NE ARG A 33 | 60.515 -6.522 124.007 1.00.56.66 | |
| ATON | 261 CZ ARG A 33 | 60.611 -7.384 125.014 1.00 58.73 | |
| ATOM | 262 NH1 ARG A 33 | 61.402 -7.121 126.045 1.00 59.32 | |
| ATOM | 263 NH2 ARG A 33 264 C ARG A 33 | 59.911 -8.511 124.991 1.00 57.91 | |
| ATOM | 264 C ARG A 33 | 62.314 -0.845 125.978 1.00 31.45 | |

Figure 18-5

| ATOM | 265 | 0 | ARG | A 33 | | 63.288 | -0.889 | 5 126.722 | 1.00 26.49 |
|--------------|------------|----------|-------|----------|---|------------------|----------------|--------------------|--------------------------|
| ATOM | 266 | N | PHE | A 34 | | 62.103 | | 5 125.123 | |
| ATOM | 267 | | | | | 63.042 | | 3 125.000 | |
| ATOM | 268 | | | | | 62.617 | | 123.858 | 1.00 31.68 |
| ATOM | 269 | | | | | 63.653 | | 2 123.486 | 1.00 29.05 |
| ATOM | 270 | | | | | 64.825 | 2.819 | 122.838 | 1.00 29.21 |
| ATOM | 271 | | | | • | 63.458 | | 123.781 | 1.00 28.25 |
| ATOM | 272 | | | | | 65.793 | | 3 122.484 | 1.00 29.35 |
| ATOM | 273 | | 2 PHE | | | 64.416 | | 123.435 | 1.00 32.67 |
| ATOM | 274 | | _ | | | 65.589 | | 3 122.783 | 1.00 29.08 |
| ATOM | 275 276 | | PHE . | | | 63.083 | 2.042 | 126.305 | 1.00 33.47 |
| ATOM ATOM | 277 | | LYS . | | · | 64.155 | | 126.852 | 1.00 27.49 |
| ATOM | 278 | | | | | 61.912 61.848 | | 126.802 | |
| ATOM | 279 | | LYS | | | 60.406 | | 128.042 128.374 | 1.00 31.48 |
| ATOM | 280 | | | A 35 | | 59.803 | | 120.374 | 1.00 30.82 1.00 32.98 |
| ATOM | 281 | CD | LYS | | | 58.404 | | 127.790 | 1.00 40.93 |
| ATOM | 282 | CE | LYS | | | 57.410 | 3.827 | | 1.00 44.56 |
| ATOM | 283 | NZ | LYS | | | 57.754 | | 128.548 | 1.00 55.10 |
| ATOM | 284 | С | LYS 2 | A 35 | | 62.443 | 2.387 | | 1.00 34.47 |
| ATOM | 285 | 0 | LYS A | A 35 | | 63.136 | 2.933 | | 1.00 32.01 |
| MOTA | 286 | N | ASP A | | | 62.180 | 1.086 | 129.190 | 1.00 36.28 |
| ATOM | 287 | CA | ASP A | | | 62.710 | 0.233 | | 1.00 37.93 |
| ATOM | 288 | CB | ASP A | | | 62.145 | | 130.126 | 1.00 41.27 |
| ATOM | 289 | CG | ASP A | | | 62.731 | | 131.157 | 1.00 43.77 |
| ATOM ATOM | 290 | OD2 | | | | 62.660 | -1.793 | | 1.00 43.92 |
| ATOM | 291 292 | C | ASP : | | | 63.261 | | 130.765 | 1.00 45.78 |
| ATOM | 293 | ō | ASP A | | | 64.227 64.902 | 0.181 | 130.174 131.201 | 1.00 38.74 |
| ATOM | 294 | N | ALA A | | | 64.760 | | 128.958 | 1.00 36.23 1.00 37.96 |
| ATOM | 295 | CA | ALA A | | | 66.201 | 0.080 | | 1.00 37.90 |
| ATOM | 296 | CB | ALA A | | | 66.525 | | 127.299 | 1.00 39.74 |
| MOTA | 297 | С | ALA A | 37 | | 66.832 | | 129.244 | 1.00 40.09 |
| MOTA | 298 | 0 | ALA A | | | 67.962 | 1:402 | | 1.00 38.80 |
| MOTA | 299 | N | MET A | | | 66.085 | 2.477 | 129.131 | 1.00 39.04 |
| ATOM | 300 | CA | MET A | | | 66.567 | 3.789 | | 1.00 38.71 |
| ATOM | 301 | CB | MET A | | | 65.965 | 4.863 | | 1.00 36.66 |
| ATOM | 302 | CG | MET A | | | 66.335 | 4.744 | | 1.00 39.16 |
| MOTA MOTA | 303 304 | SD CE | MET A | | | 68.005 | 5.298 | | 1.00 37.55 |
| ATOM | 305 | C | MET A | | | 67.892 66.187 | 7.033 4.094 | 127.287 130.995 | 1.00 35.74 |
| ATOM | 306 | ŏ | MET A | | | 66.484 | 5.173 | 131.502 | 1.00 40.58 1.00 38.12 |
| ATOM | 307 | Ŋ | ASN A | | | 65.530 | 3.147 | 131.657 | 1.00 38.12 |
| ATOM | 308 | CA | ASN A | | | 65.094 | 3.346 | | 1.00 42.46 |
| ATOM | 309 | CB | ASN A | . 39 | | 66.298 | 3.494 | 133.979 | 1.00 46.06 |
| ATOM | 310 | CG | ASN A | 39 | | 67.125 | | 134.074 | 1.00 51.69 |
| ATOM | 311 | | ASN A | | | 66.625 | 2.175 | 134.487 | 1.00 54.33 |
| MOTA | 312 | ND2 | | 39 | | 68.396 | 2 313 | 133.695 | 1.00 49.13 |
| ATOM | 313 | C | ASN A | 39 | | 64.222 | | 133.134 | 1.00 41.19 |
| ATOM | 314 | 0 | ASN A | 39 | | 64.375 | | 134.050 | 1.00 42.74 |
| ATOM | 315 | N | LEU A | 40 | | 63.301 | | 132.188 | 1.00 40.22 |
| MOTA | 316 | CA | LEU A | 40 | | 62.427 | | 132.170 | 1.00 39.85 |
| ATOM ATOM | 317 318 | CB CG | LEU A | 40 40 | | 62.524 | | 130.812 | 1.00 40.42 |
| ATOM · | 319 | | LEU A | 40 | | 63.940 63.916 | | 130.447 129.088 | 1.00 40.40 |
| ATOM | 320 | | LEU A | 40 | | 64.470 | | 131.513 | 1.00 32.75 1.00 38.89 |
| ATOM | 321 | c | LEU A | 40 | | 60.967 | | 132.505 | 1.00 38.97 |
| ATOM | 322 | ō | LEU A | 40 | | 60.076 | | 132.213 | 1.00 32.32 |
| ATOM | 323 | N | ILE A | 41 | | 60.720 | | 133.124 | 1.00 38.57 |
| ATOM | 324 | CA | ILE A | 41 | | 59.363 | | 133.520 | 1.00 42.43 |
| MOTA | 325 | CB | ILE A | 41 | | 58.536 | | 132.330 | 1.00 39.13 |
| atom | 326 | | ILE A | 41 | | 59.137 | | 131.820 | 1.00 36.51 |
| ATOM | 327 | CG1 | ILE A | 41 | | 57.082 | 3.367 | 132.774 | 1.00 38.71 |
| ATOM | 328 | | ILE A | 41 | | 56.147 | | 131.676 | 1.00 44.09 |
| ATOM | 329 | C | ILE A | 41 | | 59.376 | | 134.619 | 1.00 42.40 |
| ATCM | 330 | 0 | ILE A | 41 | | 60.255 | 2.195 | 134.654 | 1.00 43.05 |

| | ATOM | 331 N ASP A 42 | •• |
|---|--------|--------------------|--|
| | ATOM | | 58.414 3.148 135.532 1.00 47.8 |
| | ATOM | | 58.301 2.183 136.620 1 00 49 2 |
| | MOTA | 374 00 100 4 | 58.243 2.880 137.984 1.00 46.6 |
| | | A | |
| | MOTA | 101 11 42 | |
| | ATOM | 336 OD2 ASP A 42 | |
| | ATOM | 337 C ASP A 42 | 57 071 |
| | MOTA | 338 O ASP A 42 | 1.00 51.2 |
| | ATOM | 339 N GLU A 43 | 57 070 |
| | MOTA | 340 CA GLU A 43 | E 045 1.00 31.4 |
| | ATOM | 341 CB GLU A 43 | 55.945 -0.792 136.673 1.00 50.67 |
| | ATOM | 740 00 | 30.234 -2.094 137.412 1 nn 54 40 |
| | · ATOM | 747 | 33.208 -3.178 137.185 1.00 60 58 |
| | ATOM | 344 am | 55.524 -4.432 137.974 1.00 66 13 |
| | | 45 | 54.761 -5.417 137.861 1 00 70 33 |
| | ATOM | 345 - OE2 GLU A 43 | 56.536 -4.427 138.711 1.00 67.39 |
| | ATOM | 346 C GLU A 43 | |
| | ATOM | 347 O GLU A 43 | 53 55 |
| | ATOM | 348 N LYS A 44 | |
| | ATOM | 349 CA LYS A 44 | 53 534 |
| | ATOM | 350 CB LYS A 44 | E4 017 |
| | ATOM | 351 CG LYS A 44 | E2 100 J4./J |
| | ATOM | 352 CD LYS A 44 | 53 305 |
| | ATOM | 353 CE LYS A 44 | 50 11 1100 11.24 |
| | ATOM | 354 NZ LYS A 44 | 52.849 5.727 140.151 1.00 61.93 |
| | ATOM | 750 | 31.301 3.644 139.519 1.00 62 80 |
| | ATOM | 300 0 DID W dd | 34.929 2.387 137.875 1 00 44 52 |
| | ATOM | 759 | 31.732 2.701 138.052 1.00 45 31 |
| | ATOM | | 53.674 2.915 136.914 1.00 41 03 |
| | MOTA | 200 | 53.140 3.914 135.994 1 00 41 23 |
| | MOTA | 360 | 54.271 4.810 135.500 1.00 38 52 |
| | | 360 CG GLU A 45 | 54.973 5.572 136.589 1.00 40.30 |
| | MOTA | 361 CD GLU A 45 | 56.241 6.222 136.096 1.00 38.06 |
| | MOTA | 362 OE1 GLU A 45 | 57.170 5.478 135 715 1 00 36 02 |
| | ATOM | 363 OE2 GLU A 45 | |
| | MOTA | 364 C GLUA 45. | 50 450 |
| | ATOM . | 365 O GLUA 45 | E1 703 |
| | MOTA | 366 N LEUA 46 | E2 200 1101 1100 39.// |
| | ATOM | 367 CA LEU A 46 | En 100 30.90 |
| | ATOM | 368 CB LEU A 46 | En 200 |
| | ATOM | 369 CG LEU A 46 | 50 000 1.00 33.32 |
| | ATOM | 370 CD1 LEU A 46 | 70 774 |
| | ATOM | 371 CD2 LEU A 46 | 5 1.00 42.06 |
| | ATOM | 372 C LEU A 46 | 50 055 - 505 251.500 1.00 42.90 |
| | ATOM | 373 O LEU A 46 | 50 511 |
| | ATOM | 374 N ILE A 47 | 40 00 00 00 00 |
| | ATOM | 375 CA ILE A 47 | 49.861 0.718 132.928 1.00 34.03 |
| | ATOM | 376 CB ILE A 47 | 48.560 0.068 133.033 1.00 32.12 |
| | ATOM | | 47.413 1.087 132.937 1.00 32.35 |
| | ATOM | | 46.069 0.360 132,833 1.00 30.60 |
| | ATOM | | 47.448 2.015 134.156 1.00 36 56 |
| | ATOM | | 40.372 3.080 134.162 1.00 35 46 |
| | | | 48.428 -0.920 131.882 1 00 33 57 |
| | ATOM | 381 O ILE A 47 | 48.505 -0.532 130.717 1.00 27 64 |
| | MOTA | 382 N LYS A 48 | 48.231 -2.195 132.205 1.00 32.98 |
| | ATOM | 383 CA LYS A 48 | 48.102 -3.224 131.176 1.00 30.98 |
| | ATOM | 384 CB LYS A 48 | 48.038 -4.609 131.821 1.00 39.21 |
| • | ATOM | 385 CG LYS A 48 | 47.956 -5.747 130.819 1.00 46.81 |
| | ATOM | 386 CD LYS A 48 | 47.989 -7.102 131.509 1.00 50.75 |
| | ATOM | 387 CE LYS A 48 | 15 20- |
| | ATOM | 388 NZ LYS A 48 | |
| | MOTA | 389 C LYS A 48 | 46 060 1.00 50.45 |
| | ATCM | 390 C LYS A 48 | 1.00 25,55 |
| | ATOM | 391 N SER A 49 | 15 15 15 15 15 15 15 15 15 15 15 15 15 1 |
| | ATOM | 392 CA SER A 49 | 47.071 -2.992 128.996 1.00 30.69 |
| | ATOM | | 45.989 -2.802 128.033 1.00 29.32 |
| | ATOM | | 46.551 -2.805 126.609 1.00 31.53 |
| | | | 47.571 -1.834 126.443 1.00 30.74 |
| | MOTA | 395 C SER A 49 | 44.952 -3.916 128.147 1.00 31.31 |
| ٠ | atom | 396 O SER A 49 · | 45.295 -5.059 128.436 1.00 34.44 |
| | | | ··· |

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Figure 18-7

```
43.688
                                             -3:582 127.922
                                                               1.00 32.87
          397
                   ARG A
ATOM
                                    42.632
                                             -4.582 127.960
                           50
                                                               1.00 31.45
          398
                   ARG A
MOTA
               CA
MOTA
                                    41.636
                                             -4.325 129.101
                                                               1.00 28.35
          399
               CB
                   ARG A
                           50
                           50
                                    40.729
                                             -3.103 128.915
                                                               1.00 32.05
          400
               CG
                   ARG A
ATOM
                                    39.653
                                             -3.055 130.008
          401
                           50
                                                               1.00 30.46
               CD
                   ARG A
MOTA
                                                               1.00 25.21
          402
                   ARG A
                           50
                                    38.821
                                             -1.850 129.964
               NE
MOTA
                           50
                                    37.930
                                             -1.569 129.016
                                                               1.00 28.32
          403
               CZ
                   ARG A
ATOM
                                    37.726
                                             -2.406 128.001
                           50
                                                               1.00 25.45
          404
               NH1
                   ARG A
MOTA
          405
               NH2
                   ARG A
                           50
                                    37.238
                                             -0.439 129.087
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ATOM
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ATOM
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ATOM
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                           56
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ATOM
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                                    33.635
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              CB
                   GLU A
ATOM
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                                                               1.00 35.09
                                    33.474
         448
              CG
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MOTA
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                           56
                                    34.787
         449
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                                                               1.00 34.54
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                   GLU A
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ATOM
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                                                               1.00 32.35
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ATCM
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| MOTA | 465 CG LEU A 58 | 20 501 |
| ATOM | 466 CD1 LEU A 58 | 77 77 77 77 77 77 77 77 77 77 77 77 77 |
| MOTA | 467 CD2 LEU A 58 | 20 665 |
| MOTA | 468 C LEU A 58 | 20 212 |
| MOTA | 469 O LEU A 58 | 100 30.99 |
| ATOM | 470 N LEU A 59 | 27.915 0.985 118.700 1.00 35.50 |
| ATOM | 471 CA LEU A 59 | 29.733 1.279 119.993 1.00 32.55 |
| ATOM | 472 CB LEU A 59 | 29.443 2.687 120.217 1.00 30.37 |
| ATOM | 473 CG LEU A 59 | 30.387 3.279 121.268 1.00 28.01 |
| ATOM | 474 CD1 LEU A 59 | 30.174 2.828 122.716 1.00 32.19 |
| · ATOM | 475 CD2 LEU A 59 | 31.248 3.427 123.604 1.00 24.85 |
| ATOM | 476 C LEU A 59 | 28.785 3.263 123.192 1.00 25.65 |
| ATOM | 400 | 29.632 3.405 118.890 1.00 31.26 |
| ATOM | 400 | 29.020 4.442 118.652 1.00 31.80 |
| ATOM | 400 | 30.482 2.850 118.026 1.00 29.79 |
| ATOM | | 30.726 3.454 116.716 1.00 30.24 |
| MOTA | 400 | 32.131 4.055 116.637 1.00 29.99 |
| ATOM | | 32.443 4.691 115.299 1.00 28.88 |
| ATOM | 100 | 31.706 5.780 114.845 1.00 25.58 |
| ATOM | | 33.448 4.178.114.479 1.00 24.00 |
| ATOM | | 31.959 6.351 113.592 1.00 26.12 |
| ATOM | 485 CE2 PHE A 60 486 CZ PHE A 60 | 33.709 4.740 113.226 1.00 25.98 |
| ATOM | | 32.963 5.828 112.781 1.00 24.53 |
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| ATOM | 444 | 31.195 1.363 115.543 1.00 32.85 |
| ATOM | 404 | 31.075 0.418 114.431 1.00 34.59 |
| ATOM | 444 | 32.296 -0.492 114.361 1.00 32.89 |
| ATOM | | 33.576 0.238 114.116 1.00 34.25 |
| ATOM | ** * | 34.225 0.532 112.967 1.00 34.67 |
| ATOM | | 34.328 0.786 115.133 1.00 37.78 |
| ATOM | | 35.390 1.382 114.619 1.00 37.50 |
| ATOM | | 35.350 1:243 113.307 1.00 37.91 |
| ATOM | 497 C HIS A 61 498 O HIS A 61 | 29.824 -0.449 114.480 1.00 38.44 |
| ATOM | 499 N THR A 62 | 29.213 -0.612 115.538 1.00 35.78 |
| ATOM | 500 CA THR A 62 | 29.462 -1.015 113.327 1.00 39.73 |
| MOTA | 501 CB THR A 62 | 28.278 -1.868 113.218 1.00 38.05 |
| ATOM | 502 OG1 THR A 62 | 27.682 -1.825 111.804 1.00 37.22 28.631 -2.345 110.867 1.00 41 15 |
| ATOM | 503 CG2 THR A 62 | |
| ATOM | 504 C THR A 62 | 20 500 |
| ATOM | 505 O THR A 62 | 20 724 |
| ATOM | 506 N GLU A 63 | 0. 500 |
| ATOM | 507 CA GLU A 63 | 27 606 |
| MOTA | 508 CB GLU A 63 | 2.00 30.00 |
| ATOM | 509 CG GLU A 63 | 100 10.15 |
| ATOM | 510 CD GLU A 63 | 26.269 -7.451 115.171 1.00 46.90 26.472 -7.593 116.665 1.00 53.11 |
| MOTA | 511 OE1 GLU A 63 | 26 604 |
| ATOM | 512 OE2 GLU A 63 | 26.601 -8.739 117.152 1.00 52.78 26.487 -6.556 117.358 1.00 57.24 |
| ATOM | 513 C GLU A 63 | 28.320 -6.263 113.268 1.00 36.19 |
| ATOM | 514 O GLUA 63 | |
| MOTA | 515 N ASP A 64 | 25.70 |
| ATOM | 516 CA ASP A 64 | 27.755 -6.119 112.074 1.00 35.85 28.198 -6.841 110.886 1.00 37.61 |
| ATOM | 517 CB ASP A 64 | 27.363 -6.382 109.697 1.00 43.30 |
| ATOM | 518 CG ASP A 64 | 27.313 -4.872 109.582 1.00 53.38 |
| ATOM | 519 OD1 ASP A 64 | 28.290 -4.269 109.089 1.00 52.15 |
| ATOM | 520 OD2 ASP A 64 | 26.298 -4.285 110.018 1.00 53.97 |
| ATOM | 521 C ASP A 64 | 20 (22 |
| ATOM | 522 D ASP A 64 | |
| ATOM | 523 N TYR A 65 | |
| ATOM | 524 CA TYR A 65 | 30.144 -5.423 110.671 1.00 33.88 31.554 -5.153 110.419 1.00 32.91 |
| ATCM | 525 CB TYR A 65 | |
| ATOM | 526 CG TYR A 65 | |
| ATOM | 527 CD1 TYR A 65 | |
| ATOM | 528 CE1 TYR A 65 | |
| | | 35.352 -3.411 109.024 1.00 32.52 |

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Figure 18-9

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1.00 41.21

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73

GLU A

OE2

MOTA

594

42.298 -12.138 116.372

| _ | | | | | |
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| ATOM | 596 | 5 0 | GLU | A 73 | 41.957 -15.249 112.409 1.00 32.96 |
| MOTA | 597 | 7 N | ARG | | 20 700 47 |
| ATOM | 598 | | | | |
| ATOM | 599 | - | | _ | 20 540 44 |
| ATOM | 600 | | _ | | |
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| ATOM | 602 | | | | 36.366 -18.087 114.063 1.00 51.13 |
| | | | | | 35.534 -18.871 113.158 1.00 57.40 |
| MOTA | 603 | | | | 35.991 -19.870 112.403 1.00 56.36 |
| ATOM | 604 | | _ | | 37.273 -20.208 112.446 1.00 51.10 |
| ATOM | 605 | | | - | 35.172 -20.517 111.586 1.00 58.75 |
| ATOM | 606 | | ARG . | A 74 | 40.125 -17.506 112.372 1.00 43.06 |
| ATOM | 607 | | ARG . | A 74 | 40.916 -18.429 112.541 1.00 42.52 |
| MOTA | 608 | N | SER . | A 75 | 39.485 -17.305 111.222 1.00 43.63 |
| ATOM | 609 | CA | SER . | A 75 | 39.670 -18.186 110.066 1.00 44.93 |
| MOTA | 610 | CB | SER . | A 75 | 38.485 -18.089 109.113 1.00 42.05 |
| ATOM | 611 | OG | SER I | A 75 | 38.420 -16.799 108.532 1.00 38.43 |
| ATOM | 612 | С | SER A | | 40.910 -17.797 109.282 1.00 46.44 |
| ATOM | 613 | 0 | SER | | |
| ATOM | 614 | N | GLN A | | 49 466 96 999 |
| ATOM | 615 | CA | | | 40 540 |
| ATOM | 616 | CB | GLN A | | |
| ATOM | 617 | CG | GLN A | | |
| MOTA | 618 | CD | GLN A | | |
| ATOM | 619 | OE | | | 1.00 41.00 |
| ATOM | 620 | NE: | | | 44.499 -14.537 110.655 1.00 37.78 |
| | | | | | 46.669 -15.111 110.591 1.00 45.00 |
| MOTA | 621 | C | GLN A | | 42.374 -16.120 107.429 1.00 44.17 |
| ATOM | 622 | 0 | GLN A | | 43.233 -16.495 106.630 1.00 40.49 |
| MOTA | 623 | N | SER A | | 41.168 -15.713 107.053 1.00 43.11 |
| MOTA | 624 | CA | SER A | | 40.784 -15.667 105.649 1.00 44.66 |
| ATOM | 625 | CB | SER A | | 40.182 -17.004 105.220 1.00 44.56 |
| ATOM | 626 | OG | SER A | | 38.974 -17.246 105.925 1.00 42.58 |
| MOTA | 627 | С | SER A | | 39.747 -14.573 105.448 1.00 44.80 |
| ATOM | 628 | 0 | SER A | | 39.096 -14.142 106.395 1.00 45.11 |
| ATOM | 629 | N | VAL A | | 39.590 -14.137 104.207 1.00 46.06 |
| ATOM | 630 | CA | VAL A | 78 | 38.632 -13.095 103.888 1.00 47.65 |
| ATOM | 631 | CB | VAL A | . 78 | 39.107 -12.245 102.701 1.00 49.63 |
| ATOM | 632 | CG1 | L VAL A | 78 | 38.076 -11.167 102.391 1.00 51.25 |
| ATOM | 633 | CG2 | YAL A | 78 | 40.454 -11.627 103.017 1.00 53.00 |
| ATOM' | 634 | С | VAL A | 78 | 37.275 -13.682 103.530 1.00 48.07 |
| MOTA | 635 | 0 | VAL A | 78 | 37.111 -14.301 102.480 1.00 42.31 |
| MOTA | 636 | N | PRO A | 79 | 36.282 -13.492 104.407 1.00 49.82 |
| ATOM | 637 | CĐ | PRO A | 79 | 36.347 -12.782 105.696 1.00 50.81 |
| ATOM | 638 | CA | PRO A | 79 | 34.927 -13.998 104.186 1.00 51.31 |
| ATOM | 639 | CB | PRO A | 79 | 34.170 -13.450 105.396 1.00 53.13 |
| ATOM | 640 | CG | PRO A | 9 - | 35.244 -13.469 106.469 1.00 53.50 |
| ATOM | 641 | C | PRO A | ;9 | |
| ATOM | 642 | Ō | PRO A | . 9 | |
| ATOM | 643 | N | LYS A | 80 | 34.670 -12.428 102.382 1.00 55.73 33.482 -14.343 102.273 1.00 49.63 |
| ATOM | 644 | CA | LYS A | 80 | |
| ATOM | 645 | СВ | LYS A | 80 | 24 522 |
| | 646 | CG | | 80 | |
| ATOM | 647 | | LYS A | | 30.817 -14.808 99.545 1.00 56.27 |
| ATOM | | CD | LYS A | 80 | 29.586 -15.712 99.560 1.00 56.61 |
| ATOM | 648 | CE | LYS A | 80 | 28.744 -15.579 98.298 1.00 56.04 |
| ATOM | 649 | NZ | LYS A | 80 | 29.471 -16.036 97.081 1.00 58.90 |
| ATOM | 650 | C | LYS A | 80 | 32.338 -12.607 100.874 1.00 51.10 |
| ATOM | 651 | 0 | LYS A | 80 | 31.539 -12.140 101.689 1.00 49.22 |
| ATOM | 652 | N | GLY A | 81 | 32.821 -11.914 99.842 1.00 51.14 |
| ATOM | 653 | CA | GLY A | 81 | 32.418 -10.537 99.592 1.00 47.07 |
| ATOM | 654 | С | GLY A | 81 | 32.876 -9.496 100.599 1.00 46.90 |
| ATOM | 655 | 0 | GLY A | 81 | 32.671 -8.301 100.397 1.00 43.90 |
| ATOM | 656 | N | ALA A | 82 | 33.504 -9.942 101.681 1.00 44.50 |
| MOTA | 657 | CA | ALA A | 82 | 33.973 -9.029 102.715 1.00 44.69 |
| ATOM | 658 | CB | ALA A | 82 | 34.497 -9.825 103.903 1.00 44.62 |
| ATOM | 659 | С | ALA A | 82 | - 35.049 -8.073 102.215 1.00 41.82 |
| ATOM | 660 | 0 | ALA A | 82 | 35.132 -6.925 102.662 1.00 35.92 |
| | | | | | |

| ATOM | 661 | N | ARG A | 83 | 35.874 | -8.549 101.289 | 1.00 43.30 |
|------|-----|-----|-------|----|----------|---------------------------------|------------|
| ATOM | 662 | CA | ARG A | 83 | 36.959 | -7.742 100.741 | 1.00 43.25 |
| ATOM | 663 | CB | ARG A | 83 | 37.715 | -8.533 99.677 | 1.00 46.60 |
| ATOM | 664 | CG | ARG A | 83 | 38.988 | -7.865 99.222 | 1.00 51.32 |
| • | | | | | 39.636 | -8.632 98.086 | 1.00 55.55 |
| MOTA | 665 | CD | ARG A | 83 | | | |
| MOTA | 666 | NE | ARG A | 83 | 40.995 | -8.164 97.810 | |
| ATOM | 667 | CZ | ARG A | 83 | 41.330 | -6.905 97.540 | |
| ATOM | 668 | NH1 | ARG A | 83 | 40.403 | -5.954 97.504 | 1.00 62.76 |
| ATOM | 669 | NH2 | ARG A | 83 | 42.599 | -6.600 97.304 | 1.00 59.66 |
| ATOM | 670 | С | ARG A | 83 | 36.453 | -6.435 100.134 | 1.00 44.58 |
| | 671 | ō | ARG A | 83 | 37.002 | -5.365 100.395 | |
| MOTA | | | | | 35.404 | -6.528 99.323 | 1.00 41.82 |
| ATOM | 672 | N | GLU A | 84 | | | |
| MOTA | 673 | CA | GLU A | 84 | 34.824 | -5.356 98.678 | 1.00 41.44 |
| MOTA | 674 | CB | GLU A | 84 | 34.145 | -5.765 97.367 | 1.00 46.27 |
| ATOM | 675 | CG | GLU A | 84 | 33.621 | -7.185 97.388 | |
| MOTA | 676 | CD | GLU A | 84 | 34.749 | -8.198 97.308 | 1.00 54.12 |
| ATOM | 677 | | GLU A | 84 | 34.555 | ~9.344 97.764 | 1.00 59.66 |
| ATOM | 678 | OE2 | | 84 | 35.823 | -7.850 96.769 | 1.00 50.30 |
| | 679 | C | GLU A | 84 | 33.831 | -4.595 99.545 | |
| MOTA | | | | | 33.692 | -3.379 99.416 | |
| MOTA | 680 | 0 | GLU A | 84 | | | |
| MOTA | 681 | N | LYS A | 85 | 33.138 | -5.301 100.427 | 1.00 36.00 |
| MOTA | 682 | CA | LYS A | 85 | 32.154 | -4.646 101.280 | |
| ATOM | 683 | CB | LYS A | 85 | 31.089 | -5.649 101.725 | 1.00 36.60 |
| ATOM | 684 | ÇG | LYS A | 85 | 29.975 | -5.042 102.570 | 1.00 40.72 |
| ATOM | 685 | CD | LYS A | 85 | 28.939 | -6.092 102.963 | 1.00 46.21 |
| ATOM | 686 | CE | LYS A | 85 | 27.839 | -5.487 103.827 | |
| ATOM | 687 | NZ | LYS A | 85 | 26.859 | -6.513 104.287 | |
| | | | | | 32.785 | -4.008 102.513 | 1.00 36.48 |
| MOTA | 688 | c | LYS A | 85 | | | |
| ATOM | 689 | 0 | LYS A | 85 | 32.353 | -2.949 102.966 | |
| MOTA | 690 | N | TYR A | 86 | 33.819 | -4.649 103.041 | |
| ATOM | 691 | CA | TYR A | 86 | 34.468 | -4.169 104.250 | |
| ATOM | 692 | CB | TYR A | 86 | 34.410 | -5.281 105.300 | |
| ATOM | 693 | CG | TYR A | 86 | 32.990 | -5.665 105.680 | 1.00 35.09 |
| ATOM | 694 | CD1 | TYR A | 86 | . 32.165 | -4.765 106.351 | 1.00 34.06 |
| ATOM | 695 | CE1 | | 86 | 30.866 | -5.100 106.704 | |
| | 696 | CD2 | | 86 | 32.470 | -6.923 105.365 | |
| ATOM | | | | | | -7.271 105.716 | |
| MOTA | 697 | CE2 | | 86 | 31.162 | | |
| MOTA | 698 | CZ | TYR A | 86 | 30.369 | -6.350 106.386 | |
| MOTA | 699 | OH | TYR A | 86 | 29.079 | -6.658 106.738 | |
| MOTA | 700 | C . | TYR A | 86 | 35.901 | -3.672 104.046 | |
| ATOM | 701 | 0 | TYR A | 86 | 36.552 | -3.208 104.984 | |
| ATOM | 702 | N | ASN A | 87 | 36.382 | -3.777 102.814 | 1.00 36.46 |
| ATOM | 703 | CA | ASN A | 87 | 37.712 | -3.313 102.441 | 1.00 32.71 |
| ATOM | 704 | CB | ASN A | 87 | 37.768 | -1.791 102.576 | |
| | 705 | CG | ASN A | 87 | 38.989 | -1.199 101.926 | |
| MOTA | | | ASN A | 87 | 39.305 | -1.518 100.784 | |
| ATOM | 706 | | | | | -0.320 102.640 | |
| MOTA | 707 | | ASN A | 87 | 39.675 | -0.320 102.840 3.956 103.217 | |
| ATOM | 708 | С | ASN A | 87 | 38.855 | | |
| ATOM | 709 | 0 | ASN A | 87 | 39.868 | -3.315 103.512 | |
| ATOM | 710 | N | ILE A | 88 | 38.687 | -5.237 103.523 | 1.00 32.48 |
| ATOM | 711 | CA | ILE A | 88 | 39.676 | -6.018 104.248 | 1.00 33.65 |
| ATOM | 712 | CB | ILE A | 88 | 39.030 | -6.732 105.445 | 1.00 38.66 |
| | 713 | | ILE A | 88 | 40.021 | -7,680 106.081 | 1.00 41.31 |
| MOTA | | | | 88 | 38.536 | -5.707 106.461 | |
| ATOM | 714 | | | | | -4.953 107.124 | 1.00 42.25 |
| ATOM | 715 | | ILE A | 88 | 39.641 | 7 000 107 210 | 1 00 37 37 |
| ATOM | 716 | С | ILE A | 88 | 40.251 | -7.090 103.318 | |
| ATOM | 717 | 0 | ILE A | 88 | 39.555 | -7.587 102.431 | |
| ATOM | 718 | N | GLY A | 89 | 41.517 | -7.446 103.520 | |
| ATOM | 719 | CA | GLY A | 89 | 42.124 | -8.477 102.698 | |
| | 720 | C | GLY A | 89 | 43.134 | -7.994 101.675 | |
| MOTA | 721 | 0 | GLY A | 89 | 43.951 | -8.777 101.186 | |
| MOTA | 722 | | GLY A | 90 | 43.071 | -6.710 101.335 | 1.00 31.39 |
| ATOM | | N | | | | -6.158 100.371 | 1.00 23.90 |
| MOTA | 723 | CA | GLY A | 90 | 44.005 | -0.130 101 040 | 1 00 20 70 |
| ATOM | 724 | С | GLY A | 90 | 45.340 | -5.893 101.040 | 1.00 28.78 |
| MOTA | 725 | 0 | GLY A | 90 | 45.563 | -6.339 102.163 | 1.00 21.71 |
| ATOM | 726 | N | TYR A | 91 | 46.221 | -5.155 100.367 | 1.00 28.26 |
| | | | | | | | |

| MOTA | 727 CA TYR A 91 | 47.539 -4.850 100 918 1 00 32 34 |
|--------------|--------------------------------------|--|
| MOTA | 728 CB TYR A 91 | 10 177 |
| MOTA | 729 CG TYR A 91 | 40 000 7 000 |
| MOTA | 730 CD1 TYR A 91 | 48.066 -3.039 99.194 1.00 24.28 48.374 -1.829 99.822 1.00 21.55 |
| MOTA | 731 CE1 TYR A 91 | 47.970 -0.609 99.275 1.00 24.69 |
| MOTA | 732 CD2 TYR A 91 | 47.341 -2.997 98.002 1.00 24.86 |
| MOTA | 733 CE2 TYR A 91 | 46.931 -1.786 97.447 1.00 29.92 |
| ATOM | 734 CZ TYR A 91 | 47.250 -0.597 98.086 1.00 29.04 |
| ATOM | 735 OH TYR A 91 | 46.861 0.593 97.516 1.00 29.51 |
| ATOM | 736 C TYR A 91 | 47.452 -3.777 101.998 1.00 27 52 |
| MOTA | 737 O TYR A 91 | 48.314 -3.689 102.869 1 00 27 20 |
| MOTA . | 738 N GLUA 92 739 CA GLUA 92 | 46.402 -2.971 101.938 1.00 26.75 |
| ATOM | 740 | 46.232 -1.879 102.882 1.00 28.38 |
| ATOM | 741 | 45.234 -0.881 102.310 1.00 28.57 |
| MOTA | 741 CG GLU A 92 742 CD GLU A 92 | 45.232 0.471 102.982 1.00 36.94 |
| ATOM | 743 OE1 GLU A 92 | 44.178 1.395 102.396 1.00 37.40 42.999 1.293 102.794 1.00 31.29 |
| ATOM | 744 OE2 GLU A 92 | 1.00 31.22 |
| ATOM | 745 C GLU A 92 | 45 770 |
| ATOM | 746 O GLU A 92 | 46 300 |
| MOTA | 747 N. ASNA 93 | |
| MOTA | 748 CA ASN A 93 | 44.109 -3.613 105.527 1.00 24.02 |
| ATOM | 749 CB ASN A 93 | 42.727 -2.988 105.690 1.00 24.51 |
| MOTA | 750 CG ASN A 93 | 42.738 -1.488 105.405 1.00 28 61 |
| MOTA MOTA | 751 OD1 ASN A 93 752 ND2 ASN A 93 | 43.428 -0.727 106.079 1.00 25 30 |
| ATOM | 765 | 41.987 -1.063 104.393 1.00 20.45 |
| ATOM | 753 C ASN A 93 754 O ASN A 93 | 43.999 -5.132 105.407 1.00 24.79 |
| ATOM | 755 N PRO A 94 | 42.905 -5.680 105.291 1.00 21.89 |
| ATOM | 756 CD PRO A 94 | 45.142 -5.828 105.429 1.00 24.60 46.493 -5.246 105.540 1.00 22.93 |
| MOTA | 757 CA PRO A 94 | 2.00 22.00 |
| MOTA | 758 CB PRO A 94 | |
| MOTA | 759 CG PRO A 94 | 46.730 -7.488 105.093 1.00 25.46 47.299 -6.431 106.046 1.00 26.20 |
| ATOM | 760 C PRO A 94 | 44.743 -8.112 106.489 1.00 31.04 |
| ATOM | 761 O PRO A 94 | 44.411 -7.589 107.558 1.00 29 10 |
| MOTA | 762 N VAL A 95 | 44.696 -9.422 106.266 1.00 28.27 |
| ATOM ATOM | 763 CA VAL A 95 764 CB VAL A 95 | 44.299 ~10.367 107.291 1.00 28 82 |
| MOTA | 764 CB VAL A 95 765 CG1 VAL A 95 | 43.938 -11.737 106.677 1.00 30.75 |
| ATOM | 766 CG2 VAL A 95 | 43.745 -12.766 107.776 1.00 33.60 |
| ATOM | 767 C VAL A 95 | 42.679 -11.611 105.849 1.00 24.87 45.503 -10.549 108.204 1.00 29.98 |
| ATOM | 768 O VAL A 95 | |
| MOTA | 769 N SERA 96 | |
| ATOM | 770 CA SER A 96 | 45.264 -10.572 109.510 1.00 29.38 46.335 -10.766 110.485 1.00 32.56 |
| MOTA | 771 CB SER A 96 | 47.325 -9.600 110.454 1.00 34.15 |
| MOTA | 772 OG SER A 96 773 C SER A 96 | 46 758 -8.448 111.051 1 00 28 33 |
| ATOM ATOM | 224 | 45.681 -10.804 111.854 1 00 32 10 |
| ATOM | | 44 458 -10.839 111.950 1.00 37.91 |
| ATOM | 775 N TYRA 97 776 CA TYRA 97 | 46.484 -10.795 112.913 1.00 32.57 |
| ATOM | 777 CB TYR A 97 | 45.914 -10.801 114.248 1.00 34.95 |
| ATOM | 778 CG TYR A 97 | 46.685 -11.735 115.182 1.00 35.47 46.492 -13.187 114.817 1.00 40.65 |
| MOTA | 779 CD1 TYR A 97 | 46.492 -13.187 114.817 1.00 40.65 47.319 -13.812 113.882 1.00 40.63 |
| MOTA | 780 CE1 TYR A 97 | 47.319 -13.812 113.882 1.00 40.63 47.083 -15.121 113.475 1.00 42.16 |
| ATOM | 781 CD2 TYR A 97 | 45.42113.910 115.338 1.00 38.82 |
| ATOM | 782 CE2 TYR A 97 | 45.175 -15.219 114.936 1 00 42 82 |
| MOTA | 783 CZ TYR A 97 | 46.010 ~15.816 114.005 1 00 42 56 |
| ATOM | 784 OH TYRA 97 | 45.772 -17.105 113.601 1.00 46.03 |
| ATOM | 785 C TYR A 97 786 O TYR A 97 | 45.862 -9.394 114.813 1.00 37.56 |
| ATOM · | 70- | 45.601 -9.195 115.998 1.00 39.06 |
| ATOM | 787 N ALA A 98 788 CA ALA A 98 | 46.115 -8.418 113.948 1.00 31.96 |
| ATON | 789 CB ALA A 98 | 46.048 -7.024 114.341 1.00 30.43 47.105 -6.211 113.600 1.00.29.64 |
| ATOH | 790 C ALA A .98 | 0.212 220.000 1.00 23.04 |
| ATOM | 791 O ALA A 98 | 44 000 |
| ATOM | 792 N MET A 99 | 44 004 |
| | | 44.094 -7.130 112.915 1.00 30.40 |

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42.788
ATOM
         793
               CA
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                          .99
                                            -6.730 112.420
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ATOM
         794
               CB
                   MET A
                           99
                                    42.370
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                                                              1.00 30.55
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                                                              1.00 31.59
MOTA
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                           99
                                    42.052
MOTA
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               SD
                   MET
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                                    41.902
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                                                                   30.13
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ATOM -
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                                   41.703
              C
                   MET A
                           99
                                                              1.00 28.02
ATOM
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              0
                   MET A
                           99
                                   40.818
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                                                              1.00 24.53
                                   41.752
                                            -7.614 114.449
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                   PHE A 100
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MOTA
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                                                              1.00 30.47
ATOM
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                   PHE A 100
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ATOM
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              CB
                   PHE A 100
                                   39.738
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                                                   115.404
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                                                                   30..29
         803
              CG
                   PHE A 100
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MOTA
ATOM
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              CD1
                   PHE A. 100
                                   37.722
                                            -7.662 116.455
                                                              1.00 27.01
MOTA
         805
              CD2
                   PHE A 100
                                   38.756
                                            -9.506 117.575
                                                              1.00 30.68
         806
                                   36.834
                                            -7.507 117.519
                                                              1.00 31.41
MOTA
              CE1
                   PHE A 100
MOTA
         807
              CE2
                   PHE A 100
                                   37.873
                                            -9.356 118.644
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MOTA
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              CZ
                   PHE A 100
                                   36.913
                                            -8.355
                                                   118.618
                                                              1.00
                                                                   24.06
         809
                   PHE A 100
                                   41.345
                                            -7.616 116.922
                                                              1.00 29.67
              C
MOTA
                                            -6.751 117.740
ATOM
         810
              Ω
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ATOM
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ATOM
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              CB
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                                                   118.732
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MOTA
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ATOM
        814
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                                           -11.119
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              CG2
                   THR A 101
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MOTA
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                   THR A 101
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                                                              1.00
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                                                                   27.19
MOTA
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                  SER A 103
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              OG
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ATOM
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ATOM
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MOTA
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             CG2
                  THR A 107
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MOTA
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MOTA
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             O
ATOM
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        858
             N
                                   42.434
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ATCM

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| MOTA | 859 CA SER A 109 | 43.421 | 1.090 125.807 | 1 00 00 04 |
| ATOM | 860 CB SER A 109 | 44.795 | 0.910 125.160 | |
| ATOM | 861 OG SER A 109 | 45.294 | -0.310 125.160 | |
| MOTA | 862 C SER A 109 | 43.008 | -0.393 125.402 | 1.00 25.84 |
| ATOM | 863 O SER A 109 | | 2.552 125.759 | 1.00 21.13 |
| ATOM | | 43.323 | 3.312 126.672 | 1:00 23.17 |
| ATOM | | 42.311 | 2.949 124.698 | 1.00 20.83 |
| | | 41.841 | 4.327 124.583 | 1.00 21.84 |
| ATOM | 866 CB THR A 110 | 41.332 | 4.648 123.161 | 1.00 24.33 |
| ATOM | 867 OG1 THR A 110 | 42.452 | 4.769 122.276 | 1.00 25.38 |
| MOTA | 868 CG2 THR A 110 | 40.543 | 5.954 123.144 | 1.00 21.18 |
| MOTA | 869 C THR A 110 | 40.725 | 4.561 125.600 | 1.00 28.52 |
| MOTA | 870 O THR A 110 | 40.632 | 5.637 126.197 | 1.00 28.32 |
| MOTA | 871. N VAL A 111 | 39.882 | 3.558 125.809 | 1.00 28.27 |
| ATOM . | | 38.811 | 3.706 126.793 | 1.00 26.88 |
| MOTA | 873 CB VAL A 111 | 37.820 | 2.519 126.742 | 1.00 30.04 |
| MOTA | 874 CG1 VAL A 111 | 36.737 | 2.519 125.742 | 1.00 29.94 |
| MOTA | 875 CG2 VAL A 111 | 37.193 | 2.693 127.802 | 1.00 27.07 |
| ATOM | 876 C VAL A 111 | 39.440 | 2.431 125.355 | 1.00 25.26 |
| ATOM | 877 O VAL A 111 | | 3.797 128.187 | 1.00 28.10 |
| MOTA | 878 N GLN A 112 | 38.968 | 4.539 129.039 | 1.00 26.06 |
| MOTA | | 40.521 | 3.056 128.415 | 1.00 23.92 |
| ATOM | | 41.188 | 3.097 129.711 | 1.00 30.27 |
| ATOM | | 42.268 | 2.020 129.804 | 1.00 28.61 |
| | 881 CG GLN A 112 | 41.777 | 0.629 129.481 | 1.00 28.90 |
| MOTA | 882 CD GLN A 112 | 42.883 | -0.397 129.564 | 1.00 28.60 |
| MOTA | 883 OE1 GLN A 112 | 43.344 | -0.740 130.653 | 1.00 29.68 |
| MOTA | 884 NE2 GLN A 112 | 43.333 | -0.880 128.409 | 1.00 22.13 |
| ATOM | 885 C GLN A 112 | 41.834 | 4.461 129.931 | 1.00 29.99 |
| ATOM | 886 O GLN A 112 | 41.791 | 5.006 131.035 | 1.00 28.43 |
| MOTA | 887 N ALA A 113 | 42.453 | 5.004 128.885 | 1.00 28.64 |
| MOTA | 888 CA ALA A 113 | 43.083 | 6.315 129.001 | 1.00 26.62 |
| MOTA | 889 CB ALA A 113 | 43.693 | 6.732 127.684 | 1.00 23.49 |
| MOTA | 890 C ALA A 113 | 42.005 | 7.307 129.407 | 1.00 24.63 |
| ATOM | 891 O ALA A 113 | 42.232 | 8.183 130.240 | 1.00 26.38 |
| ATOM | 892 N ILE A 114 | 40.824 | 7.163 128.822 | 1.00 25.26 |
| MOTA | 893 CA ILE A 114 | 39.728 | 8.063 129.145 | |
| MOTA | 894 CB ILE A 114 | 38.554 | 7.887 128.156 | 1.00 27.05 |
| ATOM | 895 CG2 ILE A 114 | 37.387 | 8.770 128.576 | 1.00 26.93 |
| MOTA | 896 CG1 ILE A 114 | 39.008 | 8.259 126.739 | 1:00 25.86 |
| ATOM | 897 CD1 ILE A 114 | 37.938 | 8.105 125.669 | 1.00 28.38 |
| ATOM | . 898 C ILE A 114 | 39.239 | 7.823 130.578 | 1.00 28.64 |
| ATOM | 899 O ILE A 114 | 38.898 | 8.770 131.291 | 1.00 31.36 |
| ATOM | 900 N GLU A 115 | 39.210 | | 1.00 24.56 |
| ATOM | 901 CA GLU A 115 | 38.750 | | 1.00 31.17 |
| ATOM | 902 CB GLU A 115 | 38.729 | 6.257 132.358 | 1.00 32.12 |
| ATOM | 903 CG GLU A 115 | | 4.744 132.607 | 1.00 32.15 |
| ATOM | 904 CD GLU A 115 | 37.904 | 3.947 131.598 | 1.00 32.84 |
| ATOM | 905 OE1 GLU A 115 | 37.875 | 2.459 131.912 | 1.00 34.12 |
| ATOM | 906 OE2 GLU A 115 | 38.910 | 1.916 132.345 | 1.00 30.36 |
| ATOM | 907 C GLU A 115 | 36.826 | 1.827 131.699 | 1.00 31.38 |
| ATOM | | 39.675 | 6.932 133.357 | 1.00 31.65 |
| ATOM | | 39.224 | 7.446 134.383 | 1.00 29.25 |
| ATOM | | 40.970 | 6.933 133.053 | 1.00 31.50 |
| | 910 CA GLU A 116 | 41.942 | 7.564 133.934 | 1.00 32.34 |
| ATOM | 911 CB GLU A 116 | 43.367 | 7.285 133.457 | 1.00 33.29 |
| ATOM | ·912 CG GLU A 116 | 43.805 | 5.842 133.633 | 1.00 32.29 |
| atom | 913 CD GLU A 116 | 43.701 | 5.378 135.079 | 1.00 36.87 |
| ATOM | 914 OE1 GLU A 116 | 44.329 | 6.003 135.961 | 1.00 34.07 |
| MOTA | 915 OE2 GLU A 116 | 42.993 | | 1.00 35.00 |
| ATOM | 916 C GLU A 116 | 41.702 | | 1.00 36.69 |
| MOTA | 917 O GLU A 116 | 41.863 | | 1.00 34.39 |
| ATOM | 918 N PHE A 117 | 41.317 | | 1.00 31.19 |
| HOT | 919 CA PHE A 117 | | | 1.00 28.43 |
| MOT | 920 CB PHE A 117 | | | 1.00 28.43 |
| TOM | 921 CG PHE A 117 | | ' | |
| MOT | 922 CD1 PHE A 117 | | | 1.00 35.78 |
| TOM | 923 CD2 PHE A 117 | | | 1.00 33.39 |
| TOM | 924 CE1 PHE A 117 | | | 1.00 38.90 |
| • | | 10.0,2 | 5.299 131.466 | 1.00 30.65 |



| MOTA | 925 | CE2 | PHE A | 117 | 38.153 | 14.412 1 | 31.190 | 1.00 36.50 |) |
|------|-------|-----|-------|------------|--------|----------|---------|------------|---|
| MOTA | 926 | CZ | PHE A | 117 | 39.003 | 15.501 1 | .31.310 | 1.00 35.41 | |
| ATOM | 927 | С | PHE A | | 39.908 | 11.401 1 | .33.811 | 1.00 32.78 | ţ |
| | 928 | ō | PHE A | | 39.966 | 12.377 1 | | 1.00 29.82 | ! |
| MOTA | | | LEU A | | 38.874 | 10.568 1 | | 1.00 28.61 | |
| MOTA | 929 | N | | | 37.720 | 10.751 1 | | 1.00 32.00 | |
| MOTA | 930 | CA | LEU A | | | | | 1.00 32.00 | |
| MOTA | 931 | CB | LEU A | | 36.621 | 9.748 1 | | | |
| ATOM | 932 | CG | LEU A | | 36.098 | 9.830 1 | | 1.00 34.47 | |
| MOTA | 933 | | LEU A | | 34.962 | 8.836 1 | | 1.00 32.69 | |
| ATOM | 934 | CD2 | LEU A | 118 | 35.612 | 11.240 1 | | 1.00 32.24 | |
| MOTA | . 935 | С | LEU A | 118 | 38.123 | 10.590 1 | | 1.00 31.17 | |
| MOTA | 936 | 0 | LEU A | 118 | 37:576 | 11.260 1 | 36.964 | 1.00 28.32 | |
| MOTA | 937 | N | LYS A | 119 | 39.083 | 9.707 1 | .36.363 | 1.00 27.23 | , |
| ATOM | 938 | CA | LYS A | | 39.531 | 9.497 1 | 37.733 | 1.00 30.95 | j |
| | 939 | CB | LYS A | | 40.203 | 8.130 1 | 37.884 | 1.00 26.35 | j |
| ATOM | 940 | CG | LYS A | | 39.293 | 6.954 1 | | 1.00 32.44 | |
| ATOM | | CD | LYS A | | 39.895 | 5.624 1 | | 1.00 33.31 | |
| MOTA | 941 | | | | | 5.385 | | 1.00 33.47 | |
| atom | 942 | CE | LYS A | | | 4.102 1 | | 1.00 33.40 | |
| MOTA | 943 | NZ | LYS A | | 41.874 | | | 1.00 33.40 | |
| MOTA | 944 | С | LYS A | | 40.493 | 10.594 1 | | | |
| MOTA | 945 | 0 | LYS A | | 41.050 | | 139.270 | 1.00 28.83 | |
| ATOM | 946 | N | GLY A | 120 | 40.689 | | L37.308 | 1.00 33.77 | |
| ATOM | 947 | CA | GLY A | 120 | 41.571 | | 137.652 | 1.00 33.84 | |
| ATOM | 948 | С | GLY A | 120 | 43.035 | | L37.340 | 1.00 34.27 | |
| ATOM | 949 | 0 | GLY A | 120 | 43.880 | 13.227 | | 1.00 36.80 | |
| ATOM | 950 | N | ASN A | 121 | 43.347 | 11.384 1 | L36.606 | 1.00 30.77 | i |
| ATOM | 951 | CA | ASN A | | 44.731 | 11.122 1 | L36.244 | 1.00 31.73 | 5 |
| MOTA | 952 | СВ | ASN A | | 45.089 | 9.646 1 | 136.437 | 1.00 29.34 | ı |
| | 953 | CG | ASN A | | 44.856 | 9.170 | 137.851 | 1.00 35.83 | 3 |
| MOTA | 954 | | ASN A | | 45.190 | 9.861 1 | | 1.00 32.74 | ı |
| MOTA | 955 | ND2 | | | 44.304 | 7.970 1 | | 1.00 33.20 |) |
| ATOM | | | ASN A | | 44.954 | 11.506 | | 1.00 32.59 | |
| MOTA | 956 | C | | | 44.031 | 11.952 | | 1.00 34.69 | |
| MOTA | 957 | 0 | ASN A | | | | 134.322 | 1.00 32.74 | |
| ATOM | 958 | N | VAL A | | 46.186 | | L34.322 | 1.00 33.59 | |
| ATOM | 959 | CA | VAL A | | 46.540 | | | 1.00 36.09 | |
| ATOM | 960 | CB | VAL A | | 47.571 | 12.790 | | | |
| MOTA | 961 | | VAL A | | 47.884 | 13.121 | 131.438 | 1.00 37.58 | |
| ATOM | 962 | CG2 | VAL A | | 47.029 | 14.021 | | 1.00 37.19 | |
| ATOM | 963 | С | VAL A | 122 | 47.147 | | 132.352 | 1.00 34.47 | |
| ATOM | 964 | 0 | VAL A | 122 | 48.053 | 9.801 | 132.939 | 1.00 31.28 | |
| ATOM | 965 | N | ALA A | 123 | 46.646 | 9.989 | | 1.00 28.00 | |
| ATOM | 966 | CA | ALA A | 123 | 47.142 | 8.784 | 130.563 | 1.00 30.73 | |
| ATOM | 967 | CB | ALA A | | 46.133 | 7.666 | 130.727 | 1.00 32.69 | 3 |
| ATOM | 968 | С | ALA A | | 47.466 | 8.969 | 129.088 | 1.00 30.5 | 5 |
| | 969 | ō | ALA A | | 46.909 | | 128.406 | 1.00 32.89 | 9 |
| ATOM | 970 | Ŋ | PHE A | | 48.380 | | 128.613 | 1.00 27.53 | 3 |
| ATOM | 971 | CA | PHE A | | 48.807 | | 127.229 | 1.00 26.5 | |
| MOTA | | | PHE A | | 50.261 | | 127.157 | 1.00 25.33 | |
| MOTA | 972 | CB | | | 50.903 | | 125.793 | 1.00 27.84 | |
| MOTA | 973 | CG | PHE A | | | | 124.629 | 1.00 24.7 | |
| ATOM | 974 | | PHE A | | 50.179 | 8.785 | 124.025 | | |
| ATOM | 975 | CD2 | PHE A | 124 | 52.266 | 8.266 | 125.686 | 1.00 29.19 | |
| ATOM | 976 | CE1 | PHE A | | 50.802 | 8.753 | 123.385 | | |
| ATOM | 977 | CE2 | | | 52.894 | 8.235 | 124.449 | 1.00 27.3 | |
| ATOM | 978 | CZ | PHE A | 124 | 52.164 | | 123.296 | 1.00 20.93 | |
| ATOM | 979 | С | PHE A | 124 | 48.671 | | 126.675 | 1.00 21.13 | |
| ATOM | 980 | 0 | PHE A | 124 | 49.181 | | 127.260 | 1.00 25.3 | |
| MOTA | 981 | N | ASN A | | 47.933 | 6.624 | 125.580 | 1.00 18.8 | 7 |
| | 982 | CA | ASN A | | 47.750 | | 124.905 | 1.00 25.0 | |
| MOTA | 983 | CB | ASN A | | 46.271 | | 124.756 | 1.00,22.9 | |
| MOTA | | | ASN A | | 46.073 | | 123.856 | 1.00 24.0 | |
| MOTA | 984 | CG | | | 46.916 | • | 123.822 | 1.00 20.4 | |
| ATOM | 985 | ODI | ASN A | 175 175 | 44.960 | | 123.138 | 1.00 16.1 | |
| ATOM | 986 | | ASN A | | | | 123.518 | 1.00 23.4 | |
| MOTA | 987 | C | ASN A | | 48.380 | 5.410 | 122.542 | 1.00 23.4 | |
| MOTA | 988 | 0 | ASN A | 125 | 47.718 | 5.747 | 177 477 | 1.00 24.5 | |
| HOTA | 989 | N | PRO A | 126 | 49.680 | 5.103 | 123.423 | | |
| ATOM | 990 | CD | PRO A | 126 | 50.589 | 4.730 | 124.519 | 1.00 22.8 | , |
| | | | | | | | - | | |

| ATO | 4 991 CA PRO A 126 | 50.41 | ·5.130 122.160 | |
|--------------|---|--------|----------------|------------|
| ATON | 992 CB PRO A 126 | 51.829 | 4.751 122.594 | |
| ATON | | 51.56 | | |
| ATOM | | 49.867 | | |
| ATOM | | 50.173 | | |
| ATOM | | | | |
| ATOM | | 49.058 | | |
| ATOM | | 48.493 | | |
| ATOM | | 48.176 | | |
| ATOM | | 47.241 | | |
| ATOM | | 46.806 | | |
| ATOM | | 46.666 | | |
| ATOM | Th 120 | 45.461 | | |
| ATOM | - 021 7 120 | 45.732 | | 1.00 23.55 |
| ATOM | | 46.875 | | |
| ATOM | 11 122 | 44.680 | | 1.00 18.03 |
| ATOM | CD1 / 125 | 44.822 | 7.205 117.243 | 1.00 24.99 |
| ATOM | | 44.600 | | 1.00 25.11 |
| ATOM | | 44.963 | 7.293 114.857 | 1.00 24.99 |
| | 1009 N MET A 130 | 44.002 | 5.470 115.765 | 1.00 20.01 |
| ATOM | 1010 CA MET A 130 | 43.729 | 4.825 114.481 | 1.00 23.63 |
| ATOM | 1011 CB MET A 130 | 43.360 | 3.361 114.744 | 1.00 22.77 |
| ATOM | 1012 CG MET A 130 | 44.455 | 2.661 115.563 | 1.00 26.30 |
| MOTA | 1013 SD MET A 130 | 44.198 | 0.913 115.989 | 1.00 26.57 |
| ATOM | 1014 CE MET A 130 | 42.665 | 1.030 116.936 | 1.00 27.59 |
| ATOM | 1015 C MET A 130 | 42.580 | 5.617 113.869 | 1.00 23.70 |
| ATOM | 1016 O MET A 130 | 41.421 | 5.199 113.901 | 1.00 26.28 |
| ATOM | 1017 N HIS A 131 | 42.926 | 6.766 113.294 | 1.00 20.66 |
| ATOM | 1018 CA HIS A 131 | 41.933 | 7.687 112.775 | 1.00 20.99 |
| ATOM | 1019 CB HIS A 131 | 42.474 | 9.125 112.891 | 1.00 21.01 |
| ATOM | 1020 CG HIS A 131 | 43.699 | 9.391 112.069 | 1.00 28.30 |
| MOTA | 1021 CD2 HIS A 131 | 44.498 | 8.549 111.373 | 1.00 19.65 |
| MOTA | 1022 ND1 HIS A 131 | 44.246 | 10.649 111.917 | 1.00 27.76 |
| MOTA | 1023 CE1 HIS A 131 | 45.328 | 10.567 111.163 | 1.00 20.48 |
| MOTA | 1024 NE2 HIS A 131 | 45.503 | 9.302 110.820 | 1.00 24.18 |
| ATOM | 1025 C HIS A 131 | 41.280 | 7.513 111.416 | 1.00 23.76 |
| MOTA MOTA | 1026 O HIS A 131 | 40.453 | 8.341 111.051 | 1.00 21.95 |
| | 1027 N HIS A 132 | 41.600 | 6.449 110.682 | 1.00 25.12 |
| MOTA | 1028 CA HIS A 132 | 41.006 | 6.257 109.354 | 1.00 23.32 |
| ATOM | 1029 CB HIS A 132 | 42.060 | 5.715 108.388 | 1.00 17.87 |
| ATOM ATOM | 1030 CG HIS A 132 1031 CD2 HIS A 132 | 43.148 | 6.689 108.072 | 1.00 24.79 |
| ATOM | | 44.496 | 6.574 108.144 | 1.00 21.72 |
| ATOM | | 42.896 | 7.944 107.556 | 1.00 13.58 |
| ATOM | | 44.044 | 8.558 107.323 | 1.00 15.41 |
| ATOM | | 45.028 | 7.748 107.668 | 1.00 15.27 |
| ATOM | | 39.752 | 5.386 109.208 | 1.00 23.38 |
| ATOM | | 38.947 | 5.615 108.304 | 3 00 24.70 |
| ATOM | | 39.587 | 4.388 110.070 | 1.00 23.34 |
| ATOM | | 38.453 | 3.471 109.953 | 1 00 23.77 |
| ATOM | - | 38.515 | 2.417 111.053 | 1.00 27.49 |
| MOTA | 1040 C ALA A 133 1041 O ALA A 133 | 37.093 | 4.145 109.966 | 1.00 23.02 |
| ATOM | 1042 N PHE A 134 | 36.878 | 5.117 110.691 | 1.00 25.98 |
| ATOM | | 36.179 | 3.633 109.148 | 1.00 18.90 |
| ATOM | | 34.831 | 4.173 109.103 | 1.00 23.73 |
| ATOM | | 34.317 | 4.296 107.663 | 1.00 24.29 |
| | | 35.119 | 5.225 106.801 | 1.00 26.67 |
| MOTA | 1046 CD1 PHE A 134 | 36.025 | 4.724 105.867 | 1.00 28.69 |
| ATOM | 1047 CD2 PHE A 134 | 34.975 | 6.605 106.921 | 1.00 32.49 |
| MOTA | 1048 CE1 PHE A 134 | 36.775 | 5.582 105.063 | 1.00 28.65 |
| MOTA | 1049 CE2 PHE A 134 | 35.724 | 7.479 106.119 | 1.00 27.86 |
| TOM | 1050 CZ PHE A 134 | 36.623 | 6.967 105.188 | 1.00 23.93 |
| MOTA | 1051 C PHE A 134 | 33.894 | 3.260 109.884 | 1.00 25.91 |
| MOT | 1052 O PHE A 134 | 34.270 | 2.172 110.319 | 1.00 27.20 |
| MOTA | 1053 N LYS A 135 | 32.670 | 3.728 110.062 | 1.00 29.14 |
| TCM | 1054 CA LYS A 135 | 31.638 | 2.984 110.765 | 1.00 35.26 |
| TOM | 1055 CB LYS A 135 | 30.294 | 3.628 110.429 | 1.00 35.86 |
| TOM | 1056 CG LYS A 135 | 29.072 | 2.779 110.667 | 1.00 46.26 |
| | | | • | - |

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Figure 18-17

| | | | | | | 2 542 | 110.211 | 1.00 47.72 |
|--------|--------|-----|-----------|----------|--------|--------|---------|------------|
| ATOM | 1057 | CD | LYS A 13 | | 27.834 | | | 1.00 47.72 |
| ATOM | 1058 | CE | LYS A 13 | 5 | 26.610 | | 110.169 | 1.00 53.65 |
| MOTA | 1059 | NZ | LYS A 13 | 5 | 26.788 | | 109.167 | 1.00 53.27 |
| ATOM | 1060 | С | LYS A 13 | 5 | 31.617 | 1.490 | 110.414 | 1.00 35.62 |
| ATOM | 1061 | ō | LYS A 13 | | 31.609 | 0.635 | 111.301 | 1.00 32.58 |
| | 1062 | N | SER A 13 | | 31.629 | | 109.122 | 1.00 35.97 |
| ATOM- | | | | | 31.555 | -0.211 | | 1.00 38.99 |
| MOTA | 1063 | CA | SER A 13 | | | | 108.083 | 1.00 38.87 |
| ATOM | 1064 | CB | SER A 13 | | 30.172 | | | |
| MOTA | 1065 | OG | SER A 13 | 5 | 29.146 | -0.072 | | 1.00 43.54 |
| ATOM | 1066 | С | -SER A 13 | 5 | 32.608 | | 107.660 | 1.00 37.84 |
| ATOM | 1067 | 0 | SER A 13 | 5 | 32.350 | -1.491 | 106.828 | 1.00 36.33 |
| MOTA | 1068 | N | ARG A 13 | | 33.788 | -0.008 | 107.705 | 1.00 33.23 |
| | 1069 | CA | ARG A 13 | | 34.797 | -0.368 | 106.724 | 1.00 30.89 |
| MOTA | | CB | ARG A 13 | | 34.456 | | 105.385 | 1.00 33.88 |
| MOTA | 1070 | | | | 35.009 | | 104.201 | 1.00 44.41 |
| ATOM | 1071 | CG | ARG A 13 | | | | 102.880 | 1.00 46.27 |
| MOTA | 1072 | CD | ARG A 13 | | 34.809 | | | |
| MOTA | 1073 | NE | ARG A 13 | | 35.091 | | 101.768 | 1.00 48.87 |
| MOTA | 1074 | CZ | ARG A 13 | 7 | 35.352 | | 100.526 | 1.00 48.64 |
| ATOM | 1075 | NH1 | ARG A 13 | ' | 35.372 | | 100.220 | 1.00 51.82 |
| ATOM | 1076 | NH2 | ARG A 13 | 7 | 35.592 | -1.169 | 99.589 | 1.00 49.01 |
| | 1077 | C | ARG A 13 | | 36.209 | 0.021 | 107.143 | 1.00 31.84 |
| ATOM | | ō | ARG A 13 | | 36.428 | | 107.742 | 1.00 30.36 |
| MOTA | 1078 | | | | 37.166 | | 106.828 | 1.00 30.06 |
| MOTA | 1079 | N | ALA A 13 | | | | | 1.00 32.24 |
| MOTA | 1080 | CA | ALA A 13 | | 38.560 | | 107.158 | 1.00 32.24 |
| MOTA | 1081 | CB | ALA A 13 | | 39.367 | | 107.048 | |
| ATOM | 1082 | С | ALA A 13 | } | 39.095 | | 106.187 | 1.00 29.49 |
| MOTA | 1083 | 0 | ALA A 13 | 3 | 38.612 | | 105.063 | 1.00 26.11 |
| ATOM | 1084 | N | ASN A 13 | • | 40.099 | 1.206 | 106.615 | 1.00 29.54 |
| ATOM | 1085 | CA | ASN A 13 | | 40.673 | 2.241 | 105.767 | 1.00 26.99 |
| | 1086 | CB | ASN A 13 | | 39.685 | 3.415 | 105.662 | 1.00 24.10 |
| ATOM | | CG | ASN A 13 | | 40.209 | | 104.811 | 1.00 28.02 |
| ATOM | 1087 | | | | 40.729 | | 103.727 | 1.00 26.90 |
| MOTA | 1088 | | ASN A 13 | | | | 105.293 | 1.00 23.55 |
| ATOM | 1089 | ND2 | | | 40.050 | 2.703 | 105.255 | 1.00 30.17 |
| ATOM | 1090 | С | ASN A 13 | | 42.027 | | 106.285 | |
| ATOM | 1091 | 0 | ASN A 13 | , | 42.245 | 2.827 | | 1.00 27.55 |
| ATOM | 1092 | N | GLY A 14 |) | 42.944 | | 105.354 | 1.00 31.82 |
| ATOM | 1093 | CA | GLY A 14 |) | 44.277 | | 105.702 | 1.00 24.90 |
| ATOM | 1094 | С | GLY A 14 |) | 45.000 | | 106.816 | 1.00 27.79 |
| ATOM | 1095 | 0 | GLY A 14 | | 45.560 | 3.339 | 107.705 | 1.00 23.85 |
| | 1096 | N | PHE A 14 | | 45.006 | 1.365 | 106.768 | 1.00 24.35 |
| ATOM | 1097 | CA | PHE A 14 | | 45.679 | | 107.783 | 1.00 24.53 |
| MOTA | | | | | 47.031 | | 108.197 | 1.00 26.40 |
| ATOM | 1098 | CB | PHE A 14 | | 47.997 | 1 366 | 107.062 | 1.00 30.31 |
| MOTA | 1099 | CG | PHE A 14 | | | | 107.269 | 1.00 31.60 |
| MOTA | 1100 | CD1 | | | 49.145 | | | 1.00 29.44 |
| ATOM | 1101 | CD2 | PHE A 14 | | 47.781 | | 105.802 | |
| ATOM | 1102 | CE1 | PHE A 14 | L | 50.066 | | 106.243 | 1.00 30.44 |
| MOTA | 1103 - | CE2 | PHE A 14 | L | 48.694 | | 104.770 | 1.00 27.91 |
| ATOM | 1104 | CZ | PHE A 14 | L | 49.840 | 1.771 | 104.991 | 1.00 29.38 |
| MOTA | 1105 | С | PHE A 14 | L | 44.846 | 0.387 | 109.056 | 1.00 23.53 |
| MOTA | 1106 | ō | PHE A 14 | | 45.194 | | 109.941 | 1.00 23.09 |
| | 1107 | N | CYS A 14 | | 43.760 | 1.143 | 109.159 | 1.00 22.86 |
| MOTA | | | CYS A 14 | | 42.925 | | 110.356 | 1.00 23.87 |
| MOTA | 1108 | CA | | | 42.472 | 2 516 | 110.723 | 1.00 22.51 |
| MOTA | 1109 | CB | CYS A 14 | • | | 2.513 | 111.072 | 1.00 27.62 |
| MOTA | 1110 | SG | CYS A 14 | | 43.828 | 3.005 | 110 222 | 1.00 24.20 |
| ATOM | 1111 | С | CYS A 14 | | 41.694 | 0.205 | 110.233 | |
| MOTA | 1112 | 0 | CYS A 14 | ? | 40.932 | 0.307 | 109.272 | 1.00 24.12 |
| MOTA | 1113 | N | TYR A 14 | } | 41.498 | -0.663 | 111.219 | 1.00 23.84 |
| ATOM | 1114 | CA | TYR A 14 | | 40.335 | ~1.546 | 111.236 | 1.00 26.07 |
| ATOM | 1115 | CB | TYR A 14 | | 40.728 | -2.958 | 111.680 | 1.00 27.89 |
| | 1116 | CG | TYR A 14 | | 41.829 | -3.582 | 110.855 | 1.00 27.30 |
| ATOM | | CDI | TYR A 14 | ì | 43.169 | -3.329 | 111.137 | 1.00 25.76 |
| ATOM | 1117 | | TIN D -4 | <u>,</u> | 44.185 | -3 875 | 110.346 | 1.00-25.77 |
| ATOM | 1118 | CE1 | TYR A 14 | | 41.526 | _1.073 | 109.762 | 1.00 25.87 |
| MOTA | 1119 | CD2 | TYR A 14 | | | -4.394 | 108.967 | 1.00 23.10 |
| ATOM ' | 1120 | CE2 | TYR A 14 | | 42.531 | -4.741 | | 1.00 22.93 |
| ATOM | 1121 | CZ | TYR A 14 | | 43.854 | | 109.262 | 1.00 20.64 |
| ATOM | 1122 | OH | TYR A 14 | 3 | 44.849 | -5.217 | 108.476 | 1.00 20.04 |

| ATOM | | 39.281 | -0.991 112.19 | 3 1.00 24.56 |
|--------------|---|------------------|----------------------------------|--------------------------|
| MCTA | | 38.085 | -1.030 111.90 | 5 1.00 24.88 |
| ATOM | | 39.734 | -0.471 113.33 | 1 1.00 23.77 |
| MOTA | | 38.833 | 0.102 114.33 | 5 1.00 27.11 |
| ATOM | | 38.871 | -0.729 115.64 | 3 1.00 24.56 |
| ATOM | | 37.941 | | 0 1.00 23.47 |
| ATOM | | 38.430 | | 5 1.00 28.51 |
| MOTA MOTA | | 38.535 | -3.113 116.539 | |
| ATOM | | 39.248 | | |
| ATOM | | 40.428 38.277 | 1.843 114.800 | |
| ATOM | 1134 CA ASN A 145 | 38.555 | 2.453 114.669 | 1.00 22.04 |
| ATOM | 1135 CB ASN A 145 | 37.559 | 3.866 114.920 4.732 114.133 | |
| ATOM | 1136 CG ASN A 145 | 37.956 | 6.205 114.091 | 1.00 18.87 1.00 22.21 |
| ATOM | 1137 OD1 ASN A 145 | 38.223 | 6.823 115.124 | 1.00 22.21 |
| ATOM | 1138 ND2 ASN A 145 | 37.978 | 6.776 112.892 | 1.00 23.78 |
| ATCM | 1139 C ASN A 145 | 38.417 | 4.141 116.418 | 1.00 22.63 |
| MOTA | 1140 O ASN A 145 | 37.338 | 4.535 116.880 | 1.00 22.45 |
| ATOM | 1141 N ASN A 146 | 77.475 | 3.941 117.178 | 1.00 16.63 |
| MOTA | 1142 CA ASN A 146 1143 CB ASN A 146 | 39.423 | 4.160 118.628 | |
| MOTA MOTA | 1143 CB ASN A 146 1144 CG ASN A 146 | 40.708 | 3.678 119.320 | |
| ATOM | 1144 CG ASN A 146 | 41.924 | 4.508 118.967 | |
| ATOM | 1146 ND2 ASN A 146 | 42.299 42.544 | 5.421 119.704 | |
| ATOM | 1147 C ASN A 146 | 39.079 | 4.202 117.827 5.602 119.023 | |
| ATOM | 1148 O ASN A 146 | 38.452 | 5.827 120.059 | 1.00 26.32 1.00 28.34 |
| ATOM | 1149 N PRO A 147 | 39.512 | 6.605 118.231 | 1.00 28.34 |
| MOTA | 1150 CD PRO A 147 | 40.383 | 6.637 117.042 | 1.00 27.18 |
| ATOM | 1151 CA PRO A 147 | 39.150 | 7.972 118.618 | 1.00 24.15 |
| MOTA | 1152 CB PRO A 147 | 39.859 | 8.815 117.558 | 1.00 25.13 |
| MOTA MOTA | 1153 CG PRO A 147 1154 C PRO A 147 | 41.081 | 7.959 117.235 | 1.00 30.05 |
| ATOM | 1154 C PRO A 147 1155 O PRO A 147 | 37.618 | 8.136 118.578 | 1.00 26.71 |
| ATOM | 1156 N ALA A 148 | 37.017 36.989 | 8.760 119.456 7:557 117.562 | 1.00 24.93 |
| MOTA | 1157 CA ALA A 148 | 35.536 | 7:557 117.562 7.633 117.416 | 1.00 21.42 1.00 21.03 |
| MOTA | 1158 CB ALA A 148 | 35.112 | 7.044 116.072 | 1.00 21.03 |
| MOTA | 1159 C ALA A 148 | 34.838 | 6.891 118.552 | 1.00 20.49 |
| MOTA | 1160 O ALA A 148 | 33.822 | 7.344 119.067 | 1.00 21.44 |
| ATOM | 1161 N VAL A 149 | 35.381 | 5.739 118.928 | 1.00 19.20 |
| ATOM | 1162 CA VAL A 149 1163 CE VAL A 149 | 34.818 | 4.950 120.016 | 1.00 24.61 |
| ATOM ATOM | 1163 CE VAL A 149 1164 CG1 VAL A 149 | 35.570 | 3.608 120.181 | 1.00 25.96 |
| ATOM | 1165 CG2 VAL A 149 | 35.158 35.262 | 2.918 121.485 2.704 118.995 | 1.00 26.58 |
| ATOM | 1166 C VAL A 149 | 34.947 | 2.704 118.995 5.752 121.304 | 1.00 25.67 |
| ATOM | 1167 O VAL A 149 | 33.990 | 5.887 122.064 | 1.00 23.56 1.00 22.52 |
| atom | 1168 N GLY A 150 | 36.143 | 6.287 121.536 | 1.00 24.65 |
| MOTA | 1169 CA GLY A 150 | 36.390 | 7.074 122.731 | 1.00 22.82 |
| ATOM | 1170 C GLY A 150 | 35.477 | 8.281 122.838 | 1.00 25.46 |
| ATOM | 1171 O GLY A 150 1172 N ILE A 151 | 34.919 | 8.564 123.904 | 1.00 23.17 |
| ATOM ATOM | 1172 N ILE A 151 1173 CA ILE A 151 | 35.327 | 9.001 121.733 | 1.00 24.38 |
| ATOM | 1174 CB ILE A 151 | 34.481 34.610 | 10.180 121.716 | 1.00 22.85 |
| ATOM | 1175 CG2 ILE A 151 | | 10.928 120.371 12.077 120.306 | 1.00 24.45 |
| ATOM | 1176 CG1 ILE A 151 | 36.041 | 11.462 120.222 | 1.00 24.71 1.00 28.02 |
| ATOM | 1177 CD1 ILE A 151 | 36.354 | 12.056 118.854 | 1.00 27.10 |
| ATOM | 1178 C ILE A 151 | 33.018 | 9.806 121.987 | 1.00 28.19 |
| ATOM | 1179 O ILE A 151 | | 10.482 122.763 | 1.00 26.37 |
| ATOM | 1180 N GLU A 152 | 32.532 | 8.734 121.364 | 1.00 26.32 |
| ATOM | 1181 CA GLU A 152 | 31.149 | 8.314 121.601 | 1.00 30.07 |
| ATOM | 1182 CB GLU A 152 1183 CG GLU A 152 | 30.758 | 7.161 120.672 | 1.00 29.37 |
| ATOM ATOM | 1184 CD GLU A 152 | 30.609 29.455 | 7.543 119.194 8.504 118.946 | 1.00 27.68 |
| ATOM | 1185 OE1 GLU A 152 | 29.139 | 8.777 117.773 | 1.00 31.82 1.00 33.51 |
| ATOM · | 1186 OE2 GLU A 152 | 28.862 | 9.009 119.918 | 1.00 34.73 |
| ATCM | 1187 C GLU A 152 | 31.009 | 7.879 123.055 | 1.00 28.00 |
| ATOM | 1188 O GLU A 152 | 29.980 | 8.096 123.683 | 1.00 31.23 |
| | | | | - |

| | | | | | | • | | | |
|------|-------|------|---------|-------|---|------------------|--------|-----------|--------------------------|
| MOTA | 1189 | N | TYR | A 153 | | 32.054 | 7.25 | 3 123.583 | 1.00 28.72 |
| ATOM | 1190 |) CA | | A 153 | | 32.066 | | 5 124.971 | |
| ATOM | 1191 | | | A 153 | | 33.427 | | 4 125.307 | 1.00 31.56 |
| ATOM | 1192 | : CG | | A 153 | | 33.617 | | 9 126.759 | 1.00 33.17 |
| MOTA | 1193 | | | A 153 | | 33.111 | | 7 127.280 | 1.00 35.43 |
| ATOM | 1194 | | | A 153 | | 33.321 | | 128.619 | 1.00 33.52 |
| ATOM | 1195 | | | A 153 | | 34.329 | | 7 127.611 | 1.00 34.29 |
| ATOM | 1196 | | | A 153 | | 34.544 | | 128.944 | 1.00 35.34 |
| ATOM | 1197 | | | A 153 | | 34.041 | | 129.444 | 1.00 37.50 |
| ATOM | 1198 | | | A 153 | | 34.260 | | 130.767 | 1.00 37.30 |
| ATOM | 1199 | | | A 153 | | 31.828 | | 2 125.857 | 1.00 30.10 |
| ATOM | 1200 | | | A 153 | | 31.026 | | 125.037 | 1.00 32.71 |
| ATOM | 1201 | | LEU | | | 32.538 | | 125.552 | 1.00 29.14 |
| ATOM | 1202 | CA | | 1 154 | | 32.413 | | 126.310 | 1.00 23.83 |
| ATOM | 1203 | CB | LEU 2 | | | 33.477 | | 125.847 | 1.00 32.87 |
| ATOM | 1204 | CG | LEU 2 | | | 34.910 | | 126.324 | 1.00 29.68 |
| MOTA | 1205 | | LEU A | | | 35.898 | | 125.605 | 1.00 29.08 |
| ATOM | 1206 | CD | 2 LEU 2 | 154 | | 34.989 | | 127.829 | 1.00 29.29 |
| ATOM | 1207 | C. | LEU A | | | 31.020 | | 126.232 | 1.00 27.19 |
| MOTA | 1208 | ō | LEU A | | | 30.475 | | 120.232 | |
| MOTA | 1209 | N | ARG A | | | 30.443 | | 125.035 | 1.00 32.58 1.00 36.63 |
| MOTA | 1210 | CA | ARG A | | | 29.107 | | 124.869 | |
| ATOM | 1211 | CB | ARG A | | | | | 123.405 | |
| ATOM | 1212 | CG | ARG A | | | 28.661 29.581 | | 122.460 | 1.00 36.32 1.00 43.15 |
| ATOM | 1213 | CD | ARG A | | | 29.100 | | 121.023 | 1.00 43.15 |
| ATOM | 1214 | NE | ARG A | | | 27.936 | | 120.768 | 1.00 41.10 |
| ATOM | 1215 | CZ | ARG A | | | 27.331 | | 119.583 | 1.00 54.00 |
| ATOM | 1216 | | L ARG A | | | 27.772 | | 118.540 | 1.00 51.61 |
| ATOM | 1217 | | ARG A | | | 26.291 | | 119.424 | 1.00 51.76 |
| ATOM | 1218 | С | ARG A | | | 28.112 | | 125.745 | 1.00 36.25 |
| ATOM | 1219 | ō | ARG A | | | 27.270 | | 126.397 | 1.00 30.23 |
| ATOM | 1220 | N | LYS A | | | 28213 | | 125.765 | 1.00 36.48 |
| ATOM | 1221 | CA | LYS A | | | 27.315 | | 126.587 | 1.00 39.06 |
| ATOM | 1222 | CB | LYS A | | | 27.460 | | 126.256 | 1.00 41.88 |
| ATOM | 1223 | CG | LYS A | | | 26.672 | | 125.020 | 1.00 51.15 |
| ATOM | 1224 | CD | LYS A | | | 27.169 | | 123.781 | 1.00 55.56 |
| ATOM | 1225 | CE | LYS A | | | 26.117 | | 122.676 | 1.00 55.63 |
| ATOM | 1226 | NZ | LYS A | | | 24.993 | | 123.013 | 1.00 49.15 |
| ATOM | 1227 | С | LYS A | | | 27.527 | | 128.076 | 1.00 39.91 |
| MOTA | .1228 | 0 | LYS A | 156 | | 26.636 | | 128.876 | 1.00 37:01 |
| ATOM | 1229 | N | LYS A | 157 | • | 28.703 | 9.431 | 128.448 | 1.00 37.73 |
| MOTA | 1230 | CA | LYS A | 157 | | 28.985 | 9.725 | 129.847 | 1.00 36.52 |
| MOTA | 1231 | CB | LYS A | 157 | | 30.493 | 9.700 | 130.122 | 1.00 35.64 |
| ATOM | 1232 | CG | LYS A | 157 | | 31.094 | 8.308 | 130.174 | 1.00 35.44 |
| ATOM | 1233 | CD | LYS A | 157 | | 30.509 | 7.510 | 131.335 | 1.00 31.28 |
| ATOM | 1234 | CE | LYS A | 157 | | 31.077 | 6.106 | 131.388 | 1.00 31.48 |
| ATOM | 1235 | NZ | LYS A | 157 | | 30.464 | 5.310 | 132.493 | 1.00 36.39 |
| ATOM | 1236 | С | LYS A | 157 | • | 28.423 | 11.097 | 130.197 | 1.00 38.12 |
| ATOM | 1237 | 0 | LYS A | 157 | | 28.531 | 11.547 | 131.336 | 1.00 37.61 |
| MOTA | 1238 | N | GLY A | | | 27.842 | 11.768 | 129.205 | 1.00 36.27 |
| MOTA | 1239 | CA | GLY A | | | 27.257 | | 129.452 | 1.00 34.31 |
| MOTA | 1240 | С | GLY A | | | 27.972 | | 128.894 | 1.00 36.36 |
| ATOM | 1241 | 0 | GLY A | | | 27.438 | 15.399 | 128.963 | 1.00 32.96 |
| MOTA | 1242 | N | PHE A | | | 29.170 | 14.117 | 128.344 | 1.00 33.89 |
| ATOM | 1243 | CA | PHE A | | | 29.892 | 15.260 | 127.796 | 1.00 30.29 |
| ATOM | 1244 | CB | PHE A | 159 | | 31.346 | 14.892 | 127.504 | 1.00 28.62 |
| MOTA | 1245 | CG | PHE A | 159 | | 32.137 | 14.555 | 128.730 | 1.00 28.80 |
| ATOM | 1246 | CD1 | PHE A | 159 | | 32.043 | 13.300 | 129.310 | 1.00 30.41 |
| ATOM | 1247 | CD2 | PHE A | | | 32.951 | 15.513 | 129.327 | 1.00 29.37 |
| ATOM | 1248 | CE1 | PHE A | | | 32.749 | | 130.472 | 1.00 34.42 |
| MOTA | 1249 | CE2 | PHE A | | | 33.661 | | 130.488 | 1.00 31.10 |
| ATOM | 1250 | CZ | PHE A | | | 33.561 | | 131.062 | 1.00 32.32 |
| ATOM | 1251 | С | PHE A | 159 | | 29.224 | 15.786 | 126.536 | 1.00 28.88 |
| ATOM | 1252 | 0 | PHE A | 159 | | 28.765 | 15.003 | 125.705 | 1.00 27.71 |
| MOTA | 1253 | N . | LYS A | 160 | | 29.180 | 17.110 | 126.402 | 1.00 30.20 |
| ATOM | 1254 | CA | LYS A | | | 28.550 | | 125.254 | 1.00 33.98 |
| | | | | | | | | | |

Figure 18-20

| | • | |
|-------------|------------------------------|---|
| ATO: | M 1255 CB LYS A 160 | |
| ATO | 210 11 100 | 27.390 18.653 125.719 1.00 36.87 |
| ATO | | 20.273 17.914 126 419 1 00 75 |
| ATO | co 212 W 100 | 25.105 18.850 126 722 1 00 |
| | CT PI2 W 100 | 25 500 00 000 1701 1.00 48.58 |
| ATO | 112 M 100 | 25 024 10 == -27.031 1.00 30.81 |
| ATO1 | 1260 C LYS A 160 | 29.008 1.00 49.79 |
| ATON | 1261 O LYS A 160 | ~3.404 10.010 124 394 1 nn 33 En |
| ATOM | - 1910 W 100 | 29.093 19.085 123.327 1 00 30 00 |
| ATOM | | 30.700 18.846 124 857 1 00 75 |
| ATOM | ou With W 101 | |
| | cn www TOT | 31 707 00 1100 1.00 29,97 |
| ATOM | CG ANG A 161 | 20 476 |
| ATOM | 1 1266 CD ARG A 161 | 20 705 21.834 124.610 1.00 37.63 |
| ATOM | 1267 NE ARG A 161 | 23.341 124.966 1 00 30 01 |
| ATOM | | 23.303 126.341 1 00 43 76 |
| ATOM | en we with the | 30.389 23.337 127 414 3 22 |
| ATOM | wit and a 101 | 29.117 22.985 127 274 1 00 45 |
| | 1. 101 | 20 003 03 22 22 27 27 2.00 45.95 |
| ATOM | ANG M TOT | 33 000 10 10 10 10 10 43./4 |
| ATOM | 1272 O ARG A 161 | 77 700 10 12 12 1.00 32./1 |
| ATOM | 1273 N ILE A 162 | 19.090 125.092 1 00 20 52 |
| ATOM | 1274 CA ILE A 162 | 10.08/ 123.149 1 00 32 50 |
| ATOM | 201 H 102 | 34.485 17.313 123 049 1 00 00 |
| ATOM | | 34.146 15.821 122 920 1 00 00 |
| | 1276 CG2 TLE A 162 | 35 402 4 |
| ATOM | 1277 CG1 ILE A 162 | 77 147 15 1000 1.00 24.95 |
| ATOM | 1278 CD1 ILE A 162 | 32 504 4 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM | 1279 C ILE A 162 | 32.304 13.9// 123.635 1 00 34 37 |
| ATOM | 1280 O ILE A 162 | 23.333 17.810 121.886 3 NO 36 46 |
| ATOM | 1281 N LEU A 163 | 10.070 17.973 120.762 1 00 27 00 |
| MOTA | | 36.626 18.067 122.168 1 00 22 13 |
| ATOM | | 37.575 18.534 121.156 1.00 25 74 |
| ATOM | | 38.384 19.729 121 601 3 00 0 |
| | 1284 CG LEU A 163 | 30 525 20 20 20 20 20 |
| ATOM | 1285 CD1 LEU A 163 | 20 212 22 |
| ATOM | 1286 CD2 LEU A 163 | 40 361 31 31 31 31 31 31 31 31 31 31 31 31 31 |
| ATOM | 1287 C LEU A 163 | 20 547 4 |
| ATOM | 1288 O LEU A 163 | 30.34/ 1/.416 120.792 1.00 27 09 |
| ATOM | 1289 N TYR A 164 | 33.033 16.721 121.674 1 00 25 25 |
| ATOM | 1290 CA TYR A 164 | 30.000 17.237 119.496 1 00 26 07 |
| ATOM | | 39.747 16.241 119.010 1 00 26 07 |
| ATOM | 1109 | 39.021 15.181 118.179 1.00 23.38 |
| | | |
| ATOM | 1293 CD1 TYR A 164 | 40 500 21.76 |
| ATOM | 1294 CE1 TYR A 164 | 41 410 |
| ATOM | 1295 CD2 TYR A 164 | 40 202 44,90 |
| MOTA | 1296 CE2 TYR A 164 | 41 000 |
| MOTA | 1297 CZ TYR A 164 | 41.000 13.190 115.616 1.00 23 36 |
| ATOM | 1298 OH TYR A 164 | 11.003 12.235 116.426 1.00 21 50 |
| MOTA | IN A 104 | 42.506 11.296 115 878 1 00 10 41 |
| ATOM | - LN A 104 | 40.798 16.923 118.138 1.00 21.67 |
| ATOM | | |
| | 1301 N ILE A 165 | 42 052 10 10 10 19.75 |
| MOTA | 1302 CA ILE A 165 | 43 140 15 1100 25.01 |
| ATOM | 1303 CB ILE A 165 | 43 043 |
| ATOM | 1304 CG2 TLE A 165 | 46 100 20.41 |
| ATOM | 1305 CG1 ILE A 165 | 43.127 19.01/ 117.937 1.00 19.36 |
| | 1306 CD1 ILE A 165 | 13.482 119.274 1.00 23 36 |
| | A 103 | 43.003 20.402 120.299 1.00 25 05 |
| | 11 100 | 44.040 16.365 117.234 1 00 36 01 |
| | - 255 X 103 | 44.538 15.505 117.971 1.00 21.91 |
| | | |
| | 1310 CA ASP A 166 | 45 022 |
| | ¹³¹¹ CB ASP A 166 | 44 140 27.11 |
| | 1312 CG ASP A 166 | 44 600 11 12 12 13 1 1.00 28.56 |
| ATOM 1 | 1313 OD1 ASP A 166 | 45 031 13.461 113.599 1.00 34.59 |
| | 1314 OD2 ASP A 166 | 43.051 13.456 113.068 1.00 30 37 |
| | 1715 100 | 43.995 12.437 113.717 1.00 23 27 |
| | | 46.319 15.924 114.614 1 00 24 47 |
| | 310 - 301 11 100 | |
| | 317 N LEU A 167 | |
| | .318 CA LEU A 167 | 40 730 -5.55, 125.22/ 1.00 23.43 |
| | .319 CB LEU A 167 | 40 603 1.00 24.67 |
| TOM 1 | 320 CG LEU A 167 | |
| | - 550 A 207 | 49.143 17.444 116.858 1.00 26.62 |

Figure 18-21

| MOTA | 1321 | . CD1 LEU A 167 | 50.249 | 17.845 117.821 | 1.00 25.88 |
|-------|-------|-----------------|----------|----------------|------------|
| ATOM | 1322 | CD2 LEU A 167 | 48.658 | 18.668 116.092 | 1.00 22.40 |
| ATOM | 1323 | C LEU A 167 | 49.405 | 15.092 113.755 | 1.00 25.82 |
| ATOM | 1324 | | 50.504 | 15.345 113.262 | 1.00 21.89 |
| ATOM | 1325 | | 48.736 | 13.977 113.488 | 1.00 24.69 |
| | 1326 | | | | 1.00 24.59 |
| ATOM- | | | 49.244 | 12.975 112.555 | |
| ATOM | 1327 | | 48.209 | 11.852 112.410 | 1.00 27.12 |
| MOTA | 1328 | | 48.722 | 10.669 111.608 | 1.00 28.11 |
| Motā | 1329 | | 49.423 | 13.686 111.209 | 1.00 24.17 |
| ATOM | 1330 | | 48.629 | 14.559 110.865 | 1.00 17.18 |
| ATOM | 1331 | | 49.085 | 9.644 112.227 | 1.00 25.40 |
| MOTA | 1332 | OD2 ASP A 168 | 48.777 | 10.750 110.364 | 1.00 34.72 |
| MOTA | 1333 | N ALA A 169 | 50.448 | 13.312 110.446 | 1.00 21.29 |
| ATOM | 1334 | CA ALA A 169 | 50.693 | 13.927 109.140 | 1.00 25.00 |
| ATOM | 1335 | CB ALA A 169 | 52.068 | 13.498 108.601 | 1.00 21.17 |
| MOTA | 1336 | C ALA A 169 | 49.612 | 13.636 108.093 | 1.00 26.57 |
| ATOM | 1337 | O ALA A 169 | 49.641 | 14.204 107.000 | 1.00 26.90 |
| ATOM | 1338 | N HIS A 170 | 48.673 | 12.746 108.406 | 1.00 21.63 |
| MOTA | 1339 | CA HIS A 170 | 47.592 | 12.445 107.468 | 1.00 24.79 |
| | 1340 | C HIS A 170 | 46.243 | 12.867 108.045 | 1.00 20.98 |
| ATOM | 1341 | O HIS A 170 | 46.044 | 12.849 109.255 | 1.00 24.12 |
| MOTA | | | 47.550 | 10.950 107.131 | 1.00 23.17 |
| MOTA | 1342 | | | | 1.00 23.17 |
| MOTA | 1343 | CG HIS A 170 | 48.830 | 10.420 106.570 | |
| MOTA | 1344 | ND1 HIS A 170 | 49.842 | 9.982 107.385 | 1.00 31.00 |
| MOTA | 1345 | CE1 HIS A 170 | 50.825 | 9.634 106.577 | 1.00 24.33 |
| MOTA | 1346 | CD2 HIS A 170 | 49.224 | 10.329 105.273 | 1.00 22.88 |
| ATOM | 1347 | NE2 HIS A 170 | 50.502 | 9.828 105.285 | 1.00 21.89 |
| MOTA | 1348 | N HIS A 171 | 45.317 | 13.231 107.171 | 1.00 21.14 |
| ATOM | 1349 | CA HIS A 171 | 43.993 | 13.661 107.591 | 1.00 25.57 |
| MOTA | 1350 | CB HIS A 171 | 43.234 | 14.242 106.404 | 1.00 22.47 |
| ATOM | 1351 | CG HIS A 171 | 41.857 | 14.719 106.746 | 1.00 29.75 |
| ATOM | 1352 | CD2 HIS A 171 | 41.433 | 15.648 107.634 | 1.00 25.58 |
| MOTA | 1353 | ND1 HIS A 171 | 40.721 | 14.201 106.160 | 1.00 28.90 |
| ATOM | 1354 | CE1 HIS A 171 . | 39.656 | 14.787 106.676 | 1.00 25.35 |
| MOTA | 1355 | NE2 HIS A 171 | 40.060 | 15.669 107.573 | 1.00 32.40 |
| ATOM | 1356 | C HIS A 171 | 43.169 | 12.533 108.204 | 1.00 29.61 |
| ATOM | 1357 | O HIS A 171 | 43.169 | 11.411 107.698 | 1.00 27.62 |
| ATOM | 1358 | N CYS A 172 | 42.461 | 12.852 109.286 | 1.00 26.52 |
| ATOM | 1359 | CA CYS A 172 | 41.610 | 11.897 109.987 | 1.00 24.82 |
| MOTA | 1360 | CB CYS A 172 | 41.460 | 12.322 111.456 | 1.00 29.47 |
| ATOM | 1361 | SG CYS A 172 | 40.959 | 14.065 111.717 | 1.00 25.69 |
| ATOM | 1362 | C CYS A 172 | 40.237 | 11.797 109.314 | 1.00 28.21 |
| ATOM | 1363 | O CYS A 172 | 39.211 | 12.131 109.914 | 1.00 26.78 |
| ATOM | 1364 | N ASP A 173 | 40.213 | 11.332 108.066 | 1.00 22.05 |
| | 1365 | CA ASP A 173 | 38.949 | 11.217 107.350 | 1.00 27.39 |
| ATOM | 1366 | CB ASP A 173 | 39.167 | 10.646 105.931 | 1.00 30.47 |
| ATOM | 1367 | CG ASP A 173 | 39.824 | 9,264 105.922 | 1.00 29.77 |
| MOTA | 1368 | OD1 ASP A 173 | 39.886 | 8.658 104.830 | 1.00 21.14 |
| MOTA | | OD2 ASP A 173 | | 8.787 106.978 | 1.00 30.04 |
| MOTA | 1369 | | 40.288 | 10.400 108.105 | 1.00 27.86 |
| ATOM | 1370 | C ASP A 173 | 37.895 | | |
| ATOM | 1371 | O ASP A 173 | 36.720 | 10.762 108.120 | 1.00 23.47 |
| ATOM | 1372 | N GLY A 174 | 38.309 | 9.315 108.753 | 1.00 25.84 |
| MOTA | 1373 | CA GLY A 174 | 37.344 | 8.513 109.490 | 1.00 28.49 |
| ATOM | 1374. | C GLY A 174 | 36.694 | 9.296 110.619 | 1.00 26.14 |
| ATOM | 1375 | O GLY A 174 | 35.475 | 9.287 110.780 | 1.00 21.39 |
| ATOM | 1376 | N VAL A 175 | 37.510 | 9.984 111.409 | 1.00 27.24 |
| MOTA | 1377 | CA VAL A 175 | 36.995 | 10.773 112.523 | 1.00 25.53 |
| ATOM | 1378 | CB VAL A 175 | . 38.137 | 11.299 113.401 | 1.00 30.54 |
| ATOM | 1379 | CG1 VAL A 175 | 37.565 | 12.105 114.566 | 1.00 28.02 |
| ATOM | 1380 | CG2 VAL A 175 | 38.973 | 10.129 113.911 | 1.00 21.30 |
| ATOM | 1381 | C VAL A 175 | 36.163 | 11.955 112.035 | 1.00 25.01 |
| ATOM | 1382 | O VAL A 175 | 35.130 | 12.282 112.623 | 1.00 21.60 |
| | 1383 | N GLN A 176 | 36.601 | 12.594 110.957 | 1.00 25.43 |
| MOTA | 1384 | CA GLN A 176 | 35.854 | 13.730 110.426 | 1.00 26.12 |
| MOTA | 1385 | CB GLN A 176 | 36.554 | 14.336 109.205 | 1.00 24.71 |
| ATOM | 1385 | CG GLN A 176 | 35.682 | 15.349 108.469 | 1.00 26.68 |
| ATOM | 1200 | | JJ.002 | TO. 0 20 00 | |

| ` mo | 1200 | |
|--------|---------------------|--|
| OTA | 0= Can n 1/0 | 36.385 16.002 107.306 1.00 29.54 |
| ATO | 452. 21 1/0 | 37.382 16.704 107.486 1.00 26.93 |
| ATO | TIPE CENT A TIO | 35.872 15.776 106.099 1.00 27 56 |
| ATO | C OLLY M 1/0 | 34.446 13.316 110.029 1.00 27.63 |
| ATOI | - 0211 11 170 | 33.481 14.021 110.319 1.00 25 93 |
| ATOR | | 34.330 12.173 109.362 1.00 32.21 |
| ATO | | 33.027 11.696 108.915 1.00 32.72 |
| ATON | | 33.181 10.445 108.053 1 00 34 20 |
| ATON | | 31.905 10.069 107.329 1.00 39.40 |
| ATOM | | 32.060 8.819 106.497 1.00 41.42 |
| ATOM | II I I I I | 32.056 7.712 107.075 1.00 45.91 |
| ATOM | 420 11 1// | 32.206 8.947 105.264 1.00 42.35 |
| ATOM | 11 1, , | 32.128 11.377 110.099 1.00 30.54 |
| ATOM | C20 A 1// | 30.945 11.697 110.093 1.00 25.39 |
| ATOM | I 1401 N ALA A 178 | 32.707 10.750 111.114 1.00 27.03 |
| ATOM | I 1402 CA ALA A 178 | 1.00 27.03 |
| ATOM | 1403 CB ALA A 178 | |
| ATOM | 1404 C ALA A 178 | 1 |
| ATOM | | |
| ATOM | | 1.00 20.04 |
| MOTA | 1407 CA PHE A 179 | 1 |
| MOTA | 1408 CB PHE A 179 | 20 20.49 |
| ATOM | 1409 CG PHE A 179 | |
| MOTA | | |
| ATOM | 1411 CD2 PHE A 179 | |
| ATOM | 1412 CE1 PHE A 179 | |
| MOTA | 1413 CE2 PHE A 179 | |
| ATOM | 1414 CZ PHE A 179 | 1,00 20.30 |
| ATOM | 1415 C PHE A 179 | |
| ATOM | 1416 O PHE A 179 | |
| ATOM | 1417 N TYR A 180 | |
| ATOM | 1418 CA TYR A 180 | 1.00 31.00 |
| MOTA | 1419 CB TYR A 180 | 30 031 |
| MOTA | 1420 CG TYR A 180 | 2.00 33.12 |
| MOTA | 1421 CD1 TYR A 180 | 1.00 30.27 |
| ATOM | 1422 CE1 TYR A 180 | 1.00 37.31 |
| ATOM | 1423 CD2 TYR A 180 | |
| MOTA | 1424 CE2 TYR A 180 | |
| ATOM | 1425 CZ TYR A 180 | 22 000 10 201 10 - |
| ATOM | 1426 OH TYR A 180 | |
| ATOM | 1427 C TYR A 180 | 1.00 20.03 |
| ATOM | 1428 O TYR A 180 | |
| MOTA | 1429 N ASP A 181 | 20 472 |
| MOTA | 1430 CA ASP A 181 | 27 100 31.30 |
| ATOM | 1431 CB ASP A 181 | 1.00 37.30 |
| ATOM | 1432 CG ASP A 181 | 75 645 34 500 444 |
| ATOM | 1433 OD1 ASP A 181 | 26 505 12 060 440 |
| MOTA | 1434 OD2 ASP A 181 | 26.505 13.963 112.233 1.00 43.25 24.425 14.504 111.871 1.00 46.56 |
| ATOM | 1435 C ASP A 181 | 26.754 17.044 112.866 1.00 36.81 |
| ATOM | 1436 O ASP A 181 | 25.571 17.286 113.109 1.00 33.91 |
| ATOM | 1437 N THR A 182 | 27 699 17 066 112 010 |
| ATOM | 1438 CA THR A 182 | 27.327 17.412 115.184 1.00 38.27 |
| MOTA | 1439 CB THR A 182 | |
| MOTA | 1440 OG1 THR A 182 | |
| ATOM | 1441 CG2 THR A 182 | 20 000 |
| ATOM | 1442 C THR A 182 | |
| ATOM | 1443 O THR A 182 | 1.00 39.31 |
| ATOM | 1444 M ASP A 183 | 1.00 40.07 |
| atom | 1445 CA ASP A 183 | 1.00 37.01 |
| ATOM | 1446 CB ASP A 183 | 22 212 |
| ATOM | 1447 CG ASP A 183 | 76 136 71 100 33.30 |
| ATOM . | 1448 CD1 ASP A 183 | 25 (14 |
| HOTA | 1449 CD2 ASP A 183 | 75 770 70 100 110 1100 14.94 |
| TCH . | 1450 C ASP A 183 | 29 762 20 100 20.17 |
| TCM | 1451 O ASP A 183 | 20 337 |
| LTOM | 1452 N GLN A 184 | 20 500 |
| | | 28.362 18.917 119.012 1.00 35.10 |

| 3 moM | 1453 | CA | GLN A 184 | 29.030 | 18.505 120.333 | 1.00 35.16 |
|----------|------|------|-----------|--------|----------------|-------------|
| MOTA | _ | | GLN A 184 | 28.155 | 17.382 120.906 | 1.00 36.94 |
| ATOM | 1454 | | | | 17.718 120.988 | 1.00 38.34 |
| ATOM | 1455 | | GLN A 184 | 26.663 | | 1.00 43.68 |
| MOTA | 1456 | CD | GLN A 184 | 25.881 | 16.725 121.838 | |
| | 1457 | OE1 | GLN A 184 | 26.027 | 15.512 121.696 | 1.00 35.48 |
| MOTA | | | GLN A 184 | 25.036 | 17.243 122.723 | 1.00 51.06 |
| ATOM | 1458 | | | 30.479 | 18.035 120.253 | 1.00 36.32 |
| MOTA | 1459 | | GLN A 184 | _ | | 1.00 34.24 |
| ATOM | 1460 | 0 | GLN A 184 | 31.135 | | |
| ATOM | 1461 | N | VAL A 185 | 30.976 | 17.883 119.028 | 1.00 34.51 |
| | | | VAL A 185 | 32.348 | 17.443 118.804 | ·1.00 33.59 |
| ATOM | 1462 | | | 32.393 | 15.990 118.259 | 1.00 35.11 |
| MOTA | 1463 | CB | VAL A 185 | | | 1.00 23.80 |
| MOTA | 1464 | CG1 | VAL A 185 | 33.834 | | 1.00 26.00 |
| ATOM | 1465 | CG2 | VAL A 185 | 31.731 | 15.045 119.242 | |
| | 1466 | C | VAL A 185 | 33.053 | 18.354 117.803 | 1.00 33.11 |
| MOTA | | | VAL A 185 | 32.545 | 18.593 116.714 | 1.00 27.73 |
| MOTA | 1467 | 0 | | | 18.872 118.184 | 1.00 31.49 |
| ATOM | 1468 | N | PHE A 186 | 34.215 | | 1.00 30.63 |
| MOTA | 1469 | CA | PHE A 186 | 34.985 | 19.729 117.291 | |
| | 1470 | CB | PHE A 186 | 35.420 | 21.023 117.991 | 1.00 30.34 |
| ATOM | | | PHE A 186 | 36.008 | 22.047 117.051 | 1.00 30.22 |
| ATOM | 1471 | CG | | 35.265 | 23.156 116.656 | 1.00 32.23 |
| MOTA | 1472 | CD1 | PHE A 186 | 33.203 | 21.879 116.524 | 1.00 29.37 |
| ATOM | 1473 | CD2 | PHE A 186 | 37.284 | 21.079 110.324 | 1.00 27.87 |
| ATOM | 1474 | CE1 | PHE A 186 | 35.785 | 24.078 115.748 | |
| | 1475 | CE2 | PHE A 186 | 37.813 | 22.794 115.615 | 1.00 28.54 |
| MOTA | | | PHE A 186 | 37.064 | 23.892 115.227 | 1.00 30.80 |
| MOTA | 1476 | CZ | | 36.232 | 18.952 116.879 | 1.00 33.38 |
| ATOM | 1477 | С | PHE A 186 | 36.232 | | 1.00 28.30 |
| ATOM | 1478 | 0 | PHE A 186 | 36.952 | 10.0- | 1.00 32.00 |
| ATOM | 1479 | N | VAL A 187 | 36.478 | 18.877 115.574 | 1.00 32.00 |
| | 1480 | CA | VAL A 187 | 37.645 | 18.171 115.060 | 1.00 29.70 |
| MOTA | | | VAL A 187 | 37.252 | 17.095 114.019 | 1.00 30.03 |
| MOTA | 1481 | CB | | 38.510 | 16.488 113.405 | 1.00 27.77 |
| ATOM | 1482 | CG1 | VAL A 187 | | | 1.00 25.98 |
| ATOM | 1483 | CG2 | VAL A 187 | 36.410 | | 1.00 31.03 |
| MOTA | 1484 | С | VAL A 187 | 38.604 | 19.153 114.392 | |
| | 1485 | ŏ | VAL A 187 | 38.215 | 19.895 113.491 | 1.00 31.88 |
| MOTA | | | LEU A 188 | 39.850 | 19:157 114.857 | 1.00 24.88 |
| MOTA | 1486 | N | | 40.899 | 20.010 114.304 | 1.00 26.92 |
| MOTA | 1487 | CA | LEU A 188 | | 20.959 115.361 | 1.00 27.04 |
| ATOM | 1488 | CB | LEU A 188 | 41.468 | | 1.00 25.15 |
| ATOM | 1489 | CG | LEU A 188 | 42.823 | 21.565 114.963 | |
| | 1490 | | LEU A 188 | 42.686 | 22.315 113.648 | 1.00 18.53 |
| ATOM | | | LEU A 188 | 43.330 | 22.485 116.068 | 1.00 28.81 |
| MOTA | 1491 | | | 42.022 | 19.113 113.815 | 1.00 31.22 |
| ATOM | 1492 | С | LEU A 188 | | 18.333 114.587 | 1.00 25.83 |
| MOTA | 1493 | 0 | LEU A 188 | 42.579 | 10.333 114.507 | 1.00 30.53 |
| ATOM | 1494 | N | SER A 189 | 42.369 | 19.230 112.540 | 1.00 30.33 |
| | 1495 | CA | SER A 189 | 43.429 | 18.399 112.007 | 1.00 30.13 |
| ATOM | | | SER A 189 | 42.821 | 17.249 111.199 | 1.00 33.41 |
| MOTA | 1496 | CB | | 43.837 | 16.474 110.588 | 1.00 32.98 |
| MOTA | 1497 | OG | SER A 189 | | 19.120 111.143 | 1.00 27.94 |
| MOTA | 1498 | С | SER A 189 | 44.448 | | 1.00 22.14 |
| ATOM | 1499 | 0 | SER A 189 | 44.084 | | 1.00 24.80 |
| ATOM | 1500 | N | LEU A 190 | 45.728 | 18.877 11 .423 | 1.00 24.00 |
| | 1501 | CA | LEU A 190 | 46.805 | 19.438 110.614 | 1.00 22.23 |
| MOTA | | | | 47.955 | 20.000 111.459 | 1.00 23.69 |
| ATOM | | · CB | LEU A 190 | 47.733 | 21.075 112.522 | 1.00 28.92 |
| MOTA. | 1503 | CG | LEU A 190 | | | 1.00 23.01 |
| ATOM | 1504 | CD1 | LEU A 190 | 49.070 | 21.780 112.740 | 1.00 20.01 |
| | 1505 | CD2 | LEU A 190 | 46.691 | 22.093 112.087 | 1.00 28.11 |
| MOTA | | | LEU A 190 | 47.300 | 18.210 109.872 | 1.00 22.69 |
| MOTA | 1506 | C | 100 A 100 | 47.416 | 17.141 110.465 | 1.00 16.55 |
| MOTA | 1507 | 0 | LEU A 190 | - | 18.353 108.587 | 1.00 19.22 |
| ATOM | 1508 | N | HIS A 191 | 47.599 | | 1.00 23.28 |
| ATOM | 1509 | CA | HIS A 191 | 48.046 | 17.210 107.804 | |
| | 1510 | CB | HIS A 191 | 46.870 | 16.242 107.650 | |
| ATOM | | | HIS A 191 | 45.591 | 16.915 107.256 | 1.00 24.16 |
| ATOM | 1511 | CG | HT2 W T3T | 45.034 | | 1.00 17.71 |
| MOTA | 1512 | CD2 | HIS A 191 | 45.034 | 17.419 108.176 | |
| ATOM | 1513 | ND1 | HIS A 191 | 44.695 | | |
| | 1514 | CEI | HIS A 191 | 43.644 | | |
| ATOM | 1515 | VIES | HIS A 191 | 43.823 | 17.746 106.246 | 1.00 27.87 |
| ATOM | | | HIS A 191 | 48.570 | | 1.00 23.65 |
| atcm | 1516 | С | NID W IN | 48.419 | | 1.00 23.89 |
| ATOM | 1517 | 0 | HIS A 191 | | | |
| ATOM | 1518 | N | GLN A 192 | 49.209 | TP-08T T03.740 | 1.00 22.32 |
| 44 £ UAT | | | | | | |

| MOTA | 1519 | CA | GLN A | 192 | | 49.718 | 16.950 | 104.412 | 1.00 20.55 |
|-------|-------|-----|-------|------|---|--------|--------|---------|------------|
| | | | | 192 | | 50.474 | | 103.864 | 1.00 23.63 |
| ATOM | 1520 | CB | _ | | | 51.528 | | 104.797 | 1.00 24.07 |
| MOTA | 1521 | CG | GLN A | | | | | | |
| MOTA | 1522 | CD | GLN A | | | 52.110 | | 104.293 | 1.00 26.90 |
| MOTA | 1523 | OE1 | GLN A | 192 | | 52.986 | | 103.421 | 1.00 20.21 |
| ATOM | 1524 | NE2 | GLN A | 192 | | 51.605 | | 104.828 | 1.00~23.52 |
| MOTA | 1525 | С | GLN A | 192 | | 48.478 | 17.174 | 103.570 | 1.00 21.41 |
| MOTA | 1526 | ō | GLN A | | | 47.478 | | 103.726 | 1.00 20.15 |
| | | N | SER A | | | 48.528 | | 102.692 | 1.00 24.36 |
| MOTA | 1527 | | | | | 47.397 | | 101.821 | 1.00 23.98 |
| MOTA | 1528 | CA | SER A | | | | | 100.820 | 1.00 24.60 |
| MOTA | 1529 | CB | SER A | | • | 47.760 | | | |
| ATOM | 1530 | QG | SER A | 193 | | 46.729 | 19.660 | 99.861 | 1.00 25.83 |
| MOTA | 1531 | С | SER A | 193 | | 46.985 | | 101.045 | 1.00 23.74 |
| MOTA | 1532 | 0 | SER A | 193 | | 47.829 | | 100.506 | 1.00 19.80 |
| ATOM | 1533 | N· | PRO A | 194 | | 45.674 | 16.936 | 100.953 | 1.00 24.85 |
| MOTA | 1534 | CD | PRO 2 | | | 44.561 | 17.719 | 101.507 | 1.00 25.08 |
| | 1535 | CA | PRO A | | | 45.151 | 15.772 | 100.235 | 1.00 29.25 |
| ATOM | | | PRO A | | | 43.641 | | 100.444 | 1.00 30.51 |
| ATOM | 1536 | CB | | | | | | 101.758 | 1.00 30.21 |
| MOTA | 1537 | | PRO A | | | 43.554 | | | 1.00 30.75 |
| ATOM | 1538 | С | PRO A | | | 45.527 | 15.825 | 98.756 | |
| ATOM | 1539 | · Q | PRO A | | | 45.420 | 14.830 | 98.041 | 1.00 30.04 |
| MOTA | 1540 | N | GLU A | 195 | | 45.967 | 16.991 | 98.298 | 1.00 26.28 |
| MOTA | 1541 | CA | GLU F | 195 | | 46.343 | 17.127 | 96.898 | 1.00 31.11 |
| ATOM | 1542 | CB | GLU A | 195 | | 46.738 | 18.570 | 96.571 | 1.00 29.52 |
| ATOM | 1543 | CG | GLU A | | | 45.680 | 19.600 | 96.933 | 1.00 38.32 |
| ATOM | 1544 | CD | GLU A | | | 45.976 | 20.972 | 96.352 | 1.00 44.15 |
| | 1545 | | GLU A | | | 47.139 | 21.425 | 96.434 | 1.00 44.23 |
| MOTA | | | GLU A | | | | 21.605 | 95.825 | 1.00 45.06 |
| ATOM | 1546 | | | | • | 47.499 | 16.193 | 96.552 | 1.00 30.81 |
| ATOM | 1547 | C | GLU A | | | | 15.705 | 95.426 | 1.00 37.17 |
| MOTA | 1548 | 0 | GLU A | | | 47.582 | | | 1.00 25.01 |
| MOTA | 1549 | N | TYR A | | | 48.377 | 15.922 | 97.515 | |
| ATOM | 1550 | CA | TYR ? | | | 49.517 | 15.053 | 97.242 | 1.00 23.43 |
| MOTA | 1551 | CB | TYR A | 196 | | 50.810 | 15.881 | 97.223 | 1.00 26.67 |
| ATOM | 1552 | CG | TYR A | 196 | | 51.255 | 16.424 | 98.572 | 1.00 26.78 |
| ATOM | 1553 | CD1 | TYR A | -196 | | 51.957 | 15.625 | 99.476 | 1.00 26.08 |
| ATOM | 1554 | CEI | | | | 52.338 | 16.110 | 100.734 | 1.00 26.77 |
| ATOM | 1555 | CD2 | | | • | 50.944 | 17.731 | 98.958 | 1.00 27.55 |
| | 1556 | CE2 | | | | 51.320 | | 100.216 | 1.00 25.95 |
| MOTA | 1557 | CZ | TYR A | | | 52.012 | | 101.096 | 1.00 24.78 |
| MOTA | | | TYR A | | | 52.356 | | 102.345 | 1.00 25.50 |
| MOTA | 1558 | OH | | | | 49.670 | 13.906 | 98.229 | 1.00 27.05 |
| MOTA | 1559 | C | TYR A | | | | 13.088 | 98.096 | |
| MOTA | 1560 | 0 | TYR A | | | 50.585 | | 99.214 | 1.00 22.10 |
| MOTA | 1561 | N | ALA A | | | 48.785 | 13.822 | | 1.00 24.90 |
| MOTA | 1562 | CA | ALA A | | | 48.928 | | 100.199 | |
| MOTA. | 1563 | CB | ALA A | | | 49.627 | | 101.437 | 1.00 27.83 |
| ATOM | 1554 | С | ALA A | 197 | | 47.644 | | 100.608 | 1.00 26.20 |
| ATOM | 1: 65 | 0 | ALA A | 197 | | 46.553 | 12.617 | 100.484 | 1.00 22.82 |
| ATCM | 1536 | N | PHE A | 198 | | 47.795 | 10.849 | 101.102 | 1.00 31.74 |
| ATOM | 1567 | CA | PHE A | 198 | • | 46.663 | 10.072 | 101.580 | 1.00 28.74 |
| ATOM | 1568 | CB | PHE A | | | 47.130 | 8.691 | 102.036 | 1.00 30.66 |
| | 1569 | CG | | | | 46.009 | | 102.399 | 1.00 29.61 |
| MOTA | | CD1 | DME 3 | 198 | | 45.496 | 6 879 | 101.463 | 1.00 28.76 |
| ATOM | 1570 | CDI | PHE A | 100 | | 45.426 | 7 822 | 103.657 | 1.00 28.43 |
| MOTA | 1571 | CD2 | PHE A | 120 | | 44.415 | | 103.037 | 1.00 25.43 |
| MOTA | 1572 | | PHE A | 198 | | | | | |
| MOTA | 1573 | CE2 | PHE A | 198 | | 44.340 | | 103.970 | 1.00 34.62 |
| ATOM | 1574 | CZ | PHE A | 198 | | 43.837 | | 103.029 | 1.00 35.73 |
| ATOM | 1575 | С | PHE A | 198 | | 46.121 | 10.814 | 102.802 | 1.00 28.95 |
| ATOM | 1576 | ō | PHE A | 198 | | 46.892 | 11.347 | 103.596 | 1.00 25.72 |
| ATOM | 1577 | N | PRO A | 199 | | 44.792 | 10.905 | 102.941 | 1.00 28.27 |
| | 1578 | CD | PRO A | 199 | | 44.100 | 11.499 | 104.099 | 1.00 33.97 |
| ATOM | | | PRO A | 199 | | 43.813 | 10.364 | 102.008 | 1.00 32.80 |
| ATOM | 1579 | CA | PRO A | 100 | | 42.550 | 10.312 | 102.858 | 1.00-29.84 |
| ATOM | 1580 | CB | PRO A | 100 | | 42.665 | | 103.592 | 1.00 37.32 |
| MOTA | 1581 | CG | PKO A | 100 | | | | 100.965 | 1.00 35.02 |
| atom | 1582 | С | PRO A | 133 | | 43.773 | | | 1.00 48.84 |
| MOTA | 1583 | 0 | PRO A | 133 | | 44.052 | | 101.280 | |
| MOTA | 1584 | N | PHE A | 200 | | 43.441 | 11.156 | 99.734 | 1.00 33.64 |
| | | | | | | | | | |

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| | | | | | | | 00 710 | 1 00 10 11 |
|------|------|-----|--------------|-------|---------|--------|--------------|------------|
| ATOM | 1585 | CA | PHE A | 200 | 43.418 | 12.179 | 98.718 | 1.00 28.12 |
| | 1586 | CB | PHE A | 200 | 43.927 | 11.579 | 97.411 | 1.00 26.69 |
| MOTA | | | | | 45.226 | 10.833 | 97.561 | 1.00 27.33 |
| MOTA | 1587 | CG | PHE A | | | | | |
| ATOM | 1588 | CD1 | PHE A | 200 | 45.239 | 9.510 | 97.995 | 1.00 29.79 |
| | | CD2 | PHE A | | 46.439 | 11.461 | 97.302 | 1.00 24.38 |
| MOTA | 1589 | | | | | | 98.168 | 1.00 29.45 |
| ATOM | 1590 | CE1 | PHE A | 200 | 46.444 | 8.820 | | |
| ATOM | 1591 | CE2 | PHE A | 200 | 47.651 | 10.782 | 97.473 | 1.00 31.41 |
| | | | | | 47.653 | 9.458 | 97.906 | 1.00 29.64 |
| MOTA | 1592 | CZ | PHE A | | | | | 1.00 26.15 |
| MOTA | 1593 | С | PHE A | 200 ' | 42.042 | 12.795 | 98.518 | |
| - | 1594 | 0 - | PHE A | 200 | 41.935 | 13.889 | 97.986 | 1.00 27.96 |
| MOTA | | | | | 41.002 | 12.101 | 98.979 | 1.00 28.52 |
| ATOM | 1595 | N | GLU A | | | | | 1.00 35.04 |
| ATOM | 1596 | CA | GLU A | 201 | 39.614 | 12.534 | 98.806 | |
| | 1597 | CB | GLU A | 201 . | 38.695 | 11.316 | 98.810 | 1.00 33.61 |
| ATOM | | | | | 39.087 | 10.240 | 97.838 | 1.00 37.80 |
| MOTA | 1598 | CG | GLU A | | | | - | 1.00 43.48 |
| ATOM | 1599 | CD | GLU A | 201 | 38.222 | 9.016 | 97.997 | |
| | 1600 | OE1 | GLU A | 201 | 36.992 | 9.142 | 97.825 | 1.00 40.96 |
| ATOM | | | | | 38.772 | 7.937 | 98.298 | 1.00 44.17 |
| MOTA | 1601 | OE2 | GLU A | | | | | 1.00 36.30 |
| MOTA | 1602 | С | GLU A | | 39.077 | 13.516 | 99.837 | |
| | 1603 | 0 | GLU A | 201 | 38.087 | 14.206 | 99.592 | 1.00 36.47 |
| MOTA | | | | | 39.693 | 13 552 | 101.007 | 1.00 34.63 |
| ATOM | 1604 | N | LYS A | | | | | 1.00 34.09 |
| ATOM | 1605 | CA | LYS A | 202 | 39.229 | | 102.030 | |
| | 1606 | CB | LYS A | 202 | 38.294 | 13.729 | 102.992 | 1.00 40.88 |
| MOTA | | | LYS A | | 37.011 | | 102.292 | 1.00 43.17 |
| ATOM | 1607 | CG | | | | | | 1.00 47.39 |
| ATOM | 1608 | CD | LYS A | 202 | 35.935 | | 103.230 | |
| ATOM | 1609 | CE | LYS A | 202 | 34.628 | 12.663 | 102.469 | 1.00 47.74 |
| | | | LYS A | | 33.504 | 12.290 | 103.378 | 1.00 53.56 |
| MOTA | 1610 | NZ | | | | | 102.753 | 1.00 36.27 |
| ATOM | 1611 | С | LYS A | 202 | 40.382 | 15.101 | | |
| ATOM | 1612 | 0 | LYS A | 202 | 41.520 | 14.666 | 102.613 | 1.00 28.06 |
| | 1613 | N | GLY A | | 40.080 | 16.152 | 103.509 | 1.00 31.91 |
| ATOM | | | | | | | 104.228 | 1.00 33.75 |
| MOTA | 1614 | CA | GLY A | 203 | 41.115 | | | 7 |
| ATOM | 1615 | С | GLY A | 203 | 41.288 | | 103.729 | 1.00 30.54 |
| | 1616 | 0 | GLY A | | 42.174 | 18.996 | 104.200 | 1.00 28.04 |
| MOTA | | | | | 40.458 | 18.713 | 102.778 | 1.00 29.93 |
| ATOM | 1617 | N | PHE A | | | | | 1.00 35.76 |
| MOTA | 1618 | CA | PHE A | 204 | 40.557 | | 102.260 | |
| | 1619 | CB | PHE A | 204 | 39.863 | 20.217 | 100.901 | 1.00 31.41 |
| ATOM | | | | | 40.498 | 19.416 | 99.803 | 1.00 31.06 |
| ATOM | 1620 | CG | PHE A | | | | | 1.00 35.66 |
| MOTA | 1621 | CD1 | PHE A | 204 | 40.169 | 18.075 | 99.618 | |
| | 1622 | CD2 | PHE A | | 41.431 | 20.002 | 98.955 | 1.00 30.79 |
| MOTA | | | | | 40.761 | 17.329 | 98.597 | 1.00 35.20 |
| ATOM | 1623 | CEl | | | | | 97.931 | 1.00 36.08 |
| MOTA | 1624 | CE2 | PHE A | 204 | 42.033 | 19.267 | | |
| ATOM | 1625 | CZ | PHE A | 204 | 41.697 | 17.928 | 97.751 | 1.00 36.54 |
| | | c | PHE A | | 39.967 | 21.103 | 103.231 | 1.00 37.30 |
| ATOM | 1626 | | | | | 20.786 | | 1.00 33.56 |
| ATOM | 1627 | 0 | PHE A | | 39.088 | | | 1.00 38.52 |
| MOTA | 1628 | N | LEU A | 205 | 40.451 | 22.337 | | |
| | 1629 | CA | LEU A | | 40.012 | 23.427 | 103.993 | 1.00 36.81 |
| ATOM | | | | | 40.801 | 24.695 | | 1.00 34.73 |
| ATOM | 1630 | CB | LEU A | | | | | 1.00 40.98 |
| ATOM | 1631 | CG | LEU A | 205 | 40.496 | 25.954 | | |
| MOTA | 1632 | CD1 | LEU A | 205 | -40.690 | 25.677 | 105.965 | 1.00 39.87 |
| | | | LEU A | | 41.415 | 27.079 | 104.032 | 1.00 39.94 |
| ATOM | 1633 | | | | | | | 1.00 36.58 |
| ATOM | 1634 | С | LEU A | | 38.520 | 23.728 | | 1.00 40.98 |
| ATOM | 1635 | 0 | LEU A | 205 | 37.931 | 24.178 | 104.905 | |
| | | | GLU A | 206 | 37.909 | 23.477 | 102.774 | 1.00 36.07 |
| ATOM | 1636 | N | GLU A | 200 | | 23.748 | | 1.00 36.30 |
| MOTA | 1637 | CA | GLU A | ,206 | 36.486 | | | |
| ATOM | 1638 | CB | GLU A | 206 | 36.107 | 23.597 | 101.105 | 1.00 39.98 |
| | | CG | GLU A | 206 | 36.890 | 24.473 | 100.131 | 1.00 48.04 |
| MOTA | 1639 | | | | | 23.980 | | 1.00 51.87 |
| MOTE | 1640 | CD | GLU A | | 38.307 | | | 1.00 50.32 |
| ATOM | 1641 | OE1 | GLU A | 206 | 39.146 | 23.993 | 100.792 | 1.00 30.32 |
| | 1642 | OE2 | | 206 | 38.581 | 23.569 | 98.716 | 1.00 56.69 |
| ATOM | | | GLU A | 206 | 35.572 | 22.852 | | 1.00 33.85 |
| ATOM | 1643 | С | GLU A | 200 | | | | 1.00 26.22 |
| ATOM | 1644 | 3 | GLU A | 206 | 34.433 | 23.213 | | 1,00 20.22 |
| | 1645 | 11 | GLU A | 207 | 36.071 | 21.679 | | 1.00 31.68 |
| atom | | | CTI | 207 | 35.297 | 20.726 | | 1.00 31.65 |
| ATCM | 1646 | CA | GLU A | 207 | | -0.360 | 104.566 | 1.00 34.15 |
| ATOM | 1647 | CB | GLU A | 207 | 36.000 | 75.763 | TO4.300 | 1.00 22.20 |
| | 1648 | CG | GLU A | 207 | 36.044 | 18.741 | 103.179 | 1.00 33.80 |
| MOTA | | | GLU A | 207 | 37.182 | 17.751 | 103.022 | 1.00 33.85 |
| ATOM | 1649 | CD | GLU A | 207 | | 17 025 | 103.995 | 1.00 33.22 |
| ATOM | 1650 | 0E1 | GĽŲ A | 207 | 37.487 | 17.023 | 100.773 | 1.00 00.00 |
| | | | | | | | | |

| | ATOM | 1 1651 OE2 GLU A 207 | 37.76 | 0 17 600 101 0 | |
|---|--------------|--|------------------|----------------|--------------|
| | ATOM | | 35.18 | | |
| | ATOM | , | | | |
| | ATOM | | 36.00 34.15 | | |
| | ATOM | 200 | | | |
| | ATOM | | 33.96 | | |
| | ATOM | | 33.73 | | |
| | ATOM | 1658 CG1 ILE A 208 | 33.71 | | |
| | ATOM | | 34.84 | | |
| | ATOM | 1660 C ILE A 208 | 36.20 | | |
| | ATOM | 1661 O ILE A 208 | 32.82 | | |
| | ATOM | 1662 N GLY A 209 | - 32.55 | | |
| | ATOM | | 32.14 | | |
| · | | | 31.04 | | 0 1.00 33.32 |
| | ATOM | | 29.69 | | 3 1.00 37.87 |
| | MOTA | 1665 O GLY A 209 1666 N GLU A 210 | 29.579 | | 3 1.00 40.56 |
| | ATOM | | 28.67 | | 0 1.00 37.38 |
| | ATOM | 1667 CA GLU A 210 | 27.337 | | 1 1.00 42.34 |
| | MOTA | 1668 CB GLU A 210 | 27.008 | 19.012 106.82 | 3 1.00 42.73 |
| | MOTA | 1669 CG GLU A 210 | 26.860 | 17.636 107.46 | 0 1.00 47.38 |
| | MOTA | 1670 CD GLU A 210 | 26.633 | | 3 1.00 52.68 |
| | ATOM | 1671 OE1 GLU A 210 | 26.385 | | 0 1.00 50.59 |
| | MOTA | 1672 OE2 GLU A 210 | 26.711 | | 6 1.00 53.78 |
| | ATOM | 1673 C GLU A 210 | 26.287 | | 8 1.00 42 90 |
| | ATOM | 1674 O GLU A 210 | 26.516 | | 2 1.00 45 94 |
| | ATOM | 1675 N GLY A 211 | 25.130 | | 4 1.00 43.16 |
| | ATOM | 1676 CA GLY A 211 | 24.068 | | 2 1.00 43.98 |
| | ATOM | 1677 C GLY A 211 | 24.514 | | 1 1.00 45.01 |
| | MOTA | 1678 O GLY A 211 | 25.186 | | 8 1.00 48.15 |
| | MOTA | 1679 N LYS A 212 | 24.145 | | 9 1.00 41.63 |
| | MOTA | 1680 CA LYS A 212 1681 CB LYS A 212 | 24.528 | 21.495 113.32 | 8 1.00 45.07 |
| | ATOM | | 23.913 | 20.715 114.49 | 1.00 46.59 |
| | MOTA | | 22.386 | 20.591 114.462 | 2 1.00 55.31 |
| | ATOM | 1683 CD LYS A 212 | 21.651 | 21.945 114.48 | L 1.00 57.42 |
| | MOTA | 1684 CE LYS A 212 | 21.749 | 22.696 113.151 | 1.00 59.71 |
| | MOTA | 1685 NZ LYS A 212 | 21.051 | 24.017 113.178 | 3 1.00 57.43 |
| | MOTA | 1686 C LYS A 212 1687 O LYS A 212 | 26.046 | 21.513 113.469 | 1.00 42.08 |
| | MOTA | | 26.598 | 22.326 114.207 | |
| | ATOM ATOM | | 26.713 | 20.615 112.751 | |
| | ATOM | | 28.163 | 20.538 112.817 | |
| | ATOM | 1690 C GLY A 213 1691 O GLY A 213 | 28.888 | 21.519 111.916 | |
| | ATOM | 1692 N LYS A 214 | 30.122 | 21.575 111.913 | |
| | ATOM | 1693 CA LYS A 214 | 28.131 | 22.295 111.143 | |
| | ATOM | 1694 CB LYS A 214 | 28.736 | 23.274 110.250 | |
| | ATOM | 1695 CG LYS A 214 | 27.656 | 24.017 109.463 | |
| | ATOM | 1696 CD LY: A 214 | 28.189 | 25.030 108.461 | |
| | ATOM | 1697 CE LY. A 214 | 27.047 | 25.704 107.720 | |
| | ATOM | 1698 NZ LYS A 214 | 27.553 | 26.759 106.754 | |
| | ATOM | 1699 C LYS A 214 | 28.453 29.547 | 26.183 105.717 | |
| | ATOM | 1700 O LYS A 214 | | 24.259 111.085 | |
| | ATOM | 1701 N GLY A 215 | 29.002 | 24.963 111.933 | 1.00 37.92 |
| | ATOM | 1702 CA GLY A 215 | 30.851 | 24.295 110.846 | 1.00 36.57 |
| | ATOM | 1703 C GLY A 215 | 31.716 | 25.183 111.593 | 1.00 35.03 |
| | ATOM | 1704 O GLY A 215 | 32.431 | 24.448 112.709 | 1.00 34.57 |
| | ATOM | 1705 N TYR A 216 | 33.216 | 25.039 113.454 | 1.00 33.76 |
| | ATOM | 1706 CA TYR A 216 | 32.168 | 23.153 112.837 | 1.00 34.61 |
| | ATOM | 1700 CA 11R A 216 | 32.816 | 22.378 113.885 | 1.00 35.00 |
| | atom | 1708 CG TYR A 216 | 31.763 | 21.683 114.753 | 1.00 36.19 |
| | ATOM | 1709 CD1 TYR A 216 | 30.928 | 22.671 115.547 | 1.00 36.68 |
| | ATOM | 1710 CE1 TYR A 216 | 29.961 | 23.462 114.925 | 1.00 35.83 |
| | | _ | 29.249 | 24.431 115.641 | 1.00 40.89 |
| | ATOM | | 31.163 | 22.869 116.910 | 1.00 41.50 |
| | MOTA | | 30.459 | 23.834 117.634 | 1.00 40.69 |
| | ATOM | | 29.505 | 24.612 116.994 | 1.00 40.17 |
| | MOTA | | 28.816 | 25.566 117.708 | 1.00 38.09 |
| | TOM TOM | 1715 C TYR A 216 1716 O TYR A 216 | 33.877 | 21.384 113.401 | 1.00 34.05 |
| • | MOTA | 1/10 U TIK A 210 | 34.263 | 20.462 114.127 | 1.00 31.87 |
| | | | | | |

| ATOM | 1717 | 7 N | ASN A 217 | , | 34.343 | 21.580 | 112.170 | 1.00 29.90 |
|---------|------|------|-------------|------|--------|--------|-----------|-------------|
| ATOM | 1718 | 3 C2 | ASN A 217 | ri . | 35.398 | | 111.506 | 1.00 30.02 |
| | 1719 | | | | | | | 1.00 26.46 |
| MOTA | | | | | 34.833 | | 110.615 | |
| ATOM | 1720 | | | | 35.897 | | 110.105 | 1.00 30.13 |
| ATOM | 1721 | l or | | | 36.558 | 19.022 | 2 109.097 | 1.00 29.80 |
| ATOM | 1722 | NI | 2 ASN A 217 | | 36.094 | 17.659 | 110.831 | 1.00 19.92 |
| ATOM | 1723 | C | ASN A 217 | | 36.378 | | 110.915 | 1.00 30.23 |
| ATOM | 1724 | | ASN A 217 | | 35.983 | | 110.080 | 1.00 27.88 |
| | | - | LEU A 218 | | 37.565 | | | |
| MOTA | 1725 | | | | 37.655 | 21.577 | | 1.00 29.45 |
| ATOM | 1726 | | LEU A 218 | | 38.670 | 22.451 | 110.698 | 1.00 28.76 |
| MOTA | 1727 | CE | LEU A 218 | | 39.160 | 23.444 | 111.753 | 1.00 29.02 |
| ATOM | 1728 | CG | LEU A 218 | | 39.513 | 24.867 | 111.307 | 1.00 34.69 |
| MOTA | 1729 | CD | 1 LEU A 218 | • | 40.432 | 25 480 | 112.367 | 1.00 32.93 |
| ATOM | 1730 | | | | 40.197 | 24.873 | | 1.00 30.69 |
| | 1731 | | | | | | | |
| MOTA | | | LEU A 218 | | 39.870 | | 110.207 | 1.00 26.65 |
| ATOM | 1732 | | LEU A 218 | | 40.527 | | 110.999 | 1.00 25.25 |
| ATOM | 1733 | N | ASN A 219 | | 40.151 | 21.752 | 108.909 | 1.00 25.21 |
| ATOM | 1734 | CA | ASN A 219 | | 41.287 | 21.069 | 108.294 | 1.00 21.91 |
| ATOM | 1735 | CB | | | 40.875 | | 107.018 | 1.00 23.69 |
| ATOM | 1736 | | | | 39.972 | | 107.298 | 1.00 27.88 |
| | 1737 | | | | | | | |
| ATOM | | | 1 ASN A 219 | | 40.153 | | 108.289 | 1.00 29.28 |
| MOTĄ | 1738 | | | | 39.018 | | 106.407 | 1.00 24.48 |
| MOTA | 1739 | С | ASN A 219 | | 42.355 | 22.074 | 107.906 | 1.00 23.46 |
| ATOM | 1740 | 0 | ASN A 219 | | 42.059 | 23.073 | 107.259 | 1.00 28.17 |
| ATOM | 1741 | N | ILE A 220 | | 43.595 | 21.804 | 108.287 | 1.00 23.90 |
| ATOM | 1742 | CA | ILE A 220 | | 44.702 | | 107.945 | 1.00 23.22 |
| | 1743 | CB | ILE A 220 | | 45.468 | | 109.212 | 1.00 28.73 |
| ATOM | | | | | | | | |
| MOTA | 1744 | CG | | | 46.601 | | 108.831 | 1.00 26.01 |
| MOTA | 1745 | CG: | | | 44.502 | | 110.212 | 1.00 26.36 |
| ATOM | 1746 | CD: | l ILE A 220 | | 43.771 | 25.004 | 109.688 | 1.00 25.74 |
| ATOM | 1747 | С | ILE A 220 | | 45.669 | 21.929 | 107.018 | 1.00 25.29 |
| ATOM | 1748 | O | ILE A 220 | | 46.631 | | 107.477 | 1.00 20.44 |
| ATOM | 1749 | N | PRO A 221 | | 45.396 | | 105.703 | 1.00 26.34 |
| | 1750 | CD | PRO A 221 | | 44.234 | | 104.999 | 1.00 28.22 |
| MOTA | | | | | | | | |
| ATOM | 1751 | CA | PRO A 221 | | 46.271 | | 104.747 | 1.00 26.92 |
| ATOM | 1752 | CB | PRO A 221 | | 45.454 | 21.279 | | 1.00 27.81 |
| ATOM | 1753 | CG | PRO A 221 | | 44.774 | 22.622 | 103.582 | 1.00 30.62 |
| ATOM | 1754 | C | PRO A 221 | | 47.595 | 21.977 | 104.625 | 1.00 27.45 |
| ATOM | 1755 | 0 | PRO A 221 | | 47.603 | 23.199 | | 1.00 31.21 |
| ATOM | 1756 | N | LEU A 222 | | 48.704 | | 104.703 | 1.00 26.01 |
| | 1757 | CA | LEU A 222 | | 50.038 | | 104.640 | 1.00 26.41 |
| ATOM | | | | | | | | |
| ATOM | 1758 | CB | LEU A 222 | | 50.726 | | 105.997 | 1.00 26.12 |
| ATOM | 1759 | CG | LEU A 222 | | 49.960 | 22.322 | | 1.00 27.67 |
| ATOM | 1760 | CD1 | LEU A 222 | | 50.531 | 21.899 | 108.497 | 1.00 30.97 |
| ATOM | 1761 | CD2 | LEU A 222 | | 50.024 | 23.839 | 106.985 | 1.00 31.59 |
| MOTA | 1762 | С | LEU À 222 | | 50.911 | | 103.504 | 1.00 28.97 |
| MOTA | 1763 | 0 | LEU A 222 | | 50.784 | | 103.117 | 1.00 27.95 |
| | 1764 | N | PRO A 223 | | 51.821 | | 102.964 | 1.00 31.52 |
| ATOM | | | | | | | | |
| ATOM | 1765 | CD | PRO A 223 | | 52.059 | | 103.358 | 1.00 29.08 |
| ATCM | 1766 | CA | PRO A 223 | | 52.727 | | | 1.00 29.93 |
| ATOM | 1767 | CB | PRO A 223 | | 53.265 | 23.109 | 101.428 | 1.00 29.16 |
| ATOM | 1768 | CG | PRO A 223 | | 53.458 | 23.771 | 102.779 | .1.00 25.86 |
| ATOM | 1769 | C | PRO A 223 | | 53.862 | | 102.206 | 1.00 33.62 |
| | 1770 | õ | PRO A 223 | | 54.179 | | | 1.00 26.55 |
| MOTA | | | | | | | | |
| MOTA | 1771 | N | LYS A 224 | | 54.479 | | 101.153 | 1.00 34.00 |
| MOTA | 1772 | CA | LYS A 224 | | 55.595 | | 101.264 | 1.00 32.88 |
| MOTA | 1773 | CB | LYS A 224 | | 55.938 | 18.767 | 99.884 | 1.00 36.31 |
| ATOM | 1774 | CG | LYS A 224 | | 54.761 | 18.204 | 99.115 | 1.00 39.37 |
| MOTA | 1775 | CD | LYS A 224 | | 55.150 | 17.998 | 97.658 | 1.00 45.23 |
| | 1776 | CE | LYS A 224 | | 53.989 | 17.478 | 96.835 | 1.00 47.90 |
| ATOM | 1777 | | LYS A 224 | | 54.331 | | 95.388 | 1.00 46.60 |
| ATOM | | NZ | | | | 17.441 | | |
| ATOM | 1778 | C | LYS A 224 | | 56.817 | | 101.798 | 1.00 29.43 |
| MOTA | 1779 | 0 | LYS A 224 | | 56.933 | | 101.640 | 1.00 24.10 |
| ATOM | 1780 | N | GLY A 225 | | 57.735 | | 102.403 | 1.00 25.00 |
| ATCM | 1781 | CA | GLY A 225 | | 58.947 | 19.896 | 102.942 | 1.00 26.20 |
| ATOM | 1782 | C | GLY A 225 | | 58.727 | 20.792 | 104.154 | 1.00 29.44 |
| .14 411 | | - | _ | | | | _ | |

| ATOM 1 | 783 O GLY A 225 | F.O. 44.4 |
|------------|-------------------|---|
| | | 59.610 21.562 104.528 1.00 29.09 |
| | | |
| | 785 CA LEU A 226 | E7 712 E7 712 Z4.26 |
| atom 1 | 786 CB LEU A 226 | EE 020 100 100 100 25.35 |
| ATOM 1 | 787 CG LEU A 226 | 2 1.00 23.23 |
| | | 22.1/2 21./5/ 107.611 1 00.29 20 |
| | | EA COC 00 1.00 20.20 |
| | 789 CD2 LEU A 226 | E4 036 28.07 |
| ATOM 11 | 790 C LEU A 226 | EQ 333 00 1.00 2/.49 |
| | 11 220 | 30.333 21.501 106.998 1.00 24 79 |
| | - 100 A 220 | |
| | 92 N ASN A 227 | 50 554 00 1.00 20.15 |
| ATOM 17 | 93 CA ASN A 227 | 50 700 |
| ATOM 17 | 94 CB ASN A 227 | |
| | | 00.731 43.823 108 260 1 00 22 42 |
| | 22 / | |
| | 96 OD1 ASN A 227 | 50 500 07 |
| ATOM 17 | 97 ND2 ASN A 227 | 50 705 25 25 25 25 25 27 |
| ATOM 17 | 98 C ASN A 227 | 60.395 25.998 107.267 1.00 28.06 |
| ATOM 17 | - 11011 11 22 / | 59.076 22.957 109.960 1.00 23.16 |
| | | |
| ATOM 18 | 00 N ASP A 228 | 50 000 000 000 1.00 18.45 |
| ATOM 18 | 01 CA ASP A 228 | 50 250 21.29 |
| ATOM 18 | | 23.33/ 43.032 112 375 1 nn as na |
| | | 60.464 22.893 113.426 1.00 24.02 |
| | | 61 110 01 1100 24.02 |
| ATOM 180 | 04 OD1 ASP A 228 | 50 430 55 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 |
| ATOM 180 | 05 OD2 ASP A 228 | |
| ATOM 180 | 16 C 150 A 226 | 62.311 21.425 113.744 1.00 29.88 |
| | 11 620 | |
| ATOM 180 | | F7 F66 |
| ATOM 180 | 08 N ASNA 229 | |
| ATOM 180 | 9 CA ASN A 229 | |
| ATOM 181 | | 30.337 20.739 112.297 1 00 27 75 |
| | 1 22 | 59.453 27.850 111.770 1.00 32.77 |
| ATOM 181 | | 60 707 07 1.00 32.77 |
| ATOM 181 | | 1.00 30.35 |
| ATOM 181 | 3 ND2 ASN A 229 | |
| ATOM 181 | 4 C ASN A 229 | 01.000 27.691 112.053 1 00 29 11 |
| | | 57.168 26.817 111 645 1 00 70 45 |
| ATOM 181 | | |
| ATOM 181 | 6 N GLUA 230 | E7 048 60 20.75 |
| ATOM . 181 | | EE 751 |
| ATOM 181 | | 33.701 26.244 109.773 1.00 30.77 |
| | 020 11 230 | 55.929 25.716 108 341 1 00 20 11 |
| | 250 | E 6 007 00 co. |
| ATOM 1820 | | CD 110 1.00 .JJ. J4 |
| ATOM 1823 | CE1 GLU A 230 | 57 465 51.00 37.77 |
| ATOM 1822 | OE2 GLU A 230 | 57.465 24.748 106.039 1.00 38.98 |
| ATOM 1823 | | 30.33/ 20.684 105.129 1 nn 31 32 |
| | 230 | 54.723 25.407 110 527 1 00 20 12 |
| ATOM 1824 | 11 230 | 52 563 25 500 10.13 |
| ATOM 1825 | N PHE A 231 | FF 141 04 |
| ATOM 1826 | CA PHE A 231 | 2. 1.00 32.49 |
| ATOM 1827 | | 34.223 23.386 111.790 1.00 28 54 |
| | | 54.913 22.075 112.191 1.00 31.22 |
| ATOM 1828 | | |
| ATOM 1829 | CD1 PHE A 231 | 53 005 |
| ATOM 1830 | CD2 PHE A 231 | 54 076 29.06 |
| ATOM 1831 | CE1 PHE A 231 | 34.036 20.723 114.130 1.00 28 38 |
| | CDI PRE A 231 | 52.153 19.469 112.518 1.00 25.79 |
| | CE2 PHE A 231 | |
| ATOM 1833 | CZ PHE A 231 | 50 00 220.001 1.00 31.40 |
| ATOM 1834 | C PHE A 231 | E2 C22 |
| ATOM 1835 | | 33.093 24.065 113.045 1.00 26 85 |
| | | 52.483 24.092 113.277 1.00 25.99 |
| ATOM 1836 | N LEU A 232 | |
| ATOM 1837 | CA LEU A 232 | 2.00 20.75 |
| ATOM 1838 | CB LEU A 232 | 55 400 21.45 |
| ATOM 1839 | CC 150 A 232 | 33.422 25.617 115.933 1.00 25 15 |
| | CG LEU A 232 | 56.176 24.372 116 420 1 00 20 12 |
| ATOM 1840 | CD1 LEU A 232 | 20.420 1.00 28,11 |
| ATOM 1841 | CD2 LEU A 232 | |
| ATCM 1842 | C LEU A 232 | 33.208 23.540 117.328 1.00 27.87 |
| ATOM 1843 | | 33.371 26.542 114.800 1.00 26.98 |
| | O LEU A 232 | 52.449 26.866 115.544 1.00 23.34 |
| ATOM 1844 | N PHE A 233 | |
| ATOM 1845 | CA PHE A 233 | 50 050 1.00 24.99 |
| ATCM: 1846 | CB PHE A 233 | 53 540 20.13 |
| ATOM 1847 | | 33.342 29.029 112.029 1.00 30 77 |
| | CG PHE A 233 | 52.719 30.151 111.448 1.00 29.65 |
| ATOM 1948 | CD1 PHE A 233 | 20 20 20 20 20 20 20 20 20 20 20 20 20 2 |
| • | | 52.803 31.441 111.962 1.00 32.80 |
| | | |

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1.00 31.59
                                            29.903 110.412
                                    51.825
        1849
              CD2. PHE A 233
MOTA
                                            32.468 111.452
                                                              1.00 33.90
              CE1 PHE A 233
                                    52.008
        1850
MOTA
                                            30.924 109.895
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                                   51.022
        1851
              CE2
                   PHE A 233
MOTA
                                                              1.00 32.50
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                                            32.208 110.415
                   PHE A 233
              CZ
        1852
ATOM
                                    51.510
                                            27.999 113.031
                                                              1.00 31.62
                   PHE A 233
        1853
              С
ATOM
                                            28.603 113.532
                                                              1.00 25.88
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                   PHE A 233
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ATOM
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                                    51.370
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                   ALA A 234
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              N
MOTA
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        1856
              CA
                   ALA A 234
MOTA
                                                              1.00 20.08
                                            25.279 110.864
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              CB
ATOM
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MOTA
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MOTA
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                   LEU A 235
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                                            25.285
        1860
              N
MOTA
                   LEU A 235
                                    49.367
                                            24.781 115.195
                                                              1.00 33.70
MOTA
        1861
              CA
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| ATOM | 1982 | OE2 | GĻU A | 249 | 30 | .252 | 19.609 | 129.620 | 1.00 38.57 |
| ATOM | 1983 | C | GLU A | | | .995 | 19.119 | 128.623 | 1.00 32.30 |
| | 1984 | ō | GLU A | | | .472 | 18 884 | 129.728 | 1.00 28.51 |
| MOTA | | | VAL A | | | .434 | 18 547 | 127.502 | 1.00 33.74 |
| MOTA | 1985 | N | | | | | | 127.494 | 1.00 29.31 |
| ATOM. | 1986 | CA | VAL A | | | .516 | 16 174 | 127.926 | 1.00 29.85 |
| ATOM | 1987 | CB | VAL A | | _ | .988 | | | 1.00 24.36 |
| MOTA | 1988 | | VAL A | | | .908 | | 126.958 | |
| ATOM | 1989 | CG2 | VAL A | 250 | | 3.121 | | 127.978 | 1.00 25.60 |
| ATOM | 1990 | C· | _VAL A | 250 | 38 | 3.066 | | 126.076 | 1.00 29.30 |
| ATOM | 1991 | 0 | VAL A | 250 | 37 | .358 | 17.741 | 125.114 | 1.00 24.46 |
| ATOM | 1992 | N | TYR A | 251 | 39 | .323 | | 125.930 | 1.00 27.96 |
| MOTA | 1993 | CA | TYR A | | . 39 | .865 | 16.913 | 124.585 | 1.00 30.06 |
| | 1994 | CB | TYR A | | | .585 | 18.206 | 124.165 | 1.00 25.89 |
| ATOM | 1995 | CG | TYR A | | | .998 | 18.370 | 124.692 | 1.00 29.90 |
| ATOM | 1996 | | TYR A | | | .087 | | 124.029 | 1.00 26.02 |
| MOTA | | CE1 | | | | 1.390 | 17 953 | 124.507 | 1.00 29.20 |
| ATOM | 1997 | | | | | .249 | | 125.849 | 1.00 31.96 |
| MOTA | 1998 | CD2 | | | | | | 126.338 | 1.00 31.54 |
| MOTA | 1999 | CE2 | | | | 3.551 | | | 1.00 31.46 |
| MOTA | 2000 | CZ | TYR A | | | 1.614 | | 125.664 | 1.00 31.40 |
| ATOM | 2001 | ОН | TYR A | | | .894 | | 126.152 | |
| MOTA | 2002 | С | TYR A | | | .801 | | 124.451 | 1.00 27.56 |
| ATOM | 2003 | 0 | TYR A | 251 | 41 | .382 | | 125.436 | 1.00 28.23 |
| ATOM | 2004 | N | LEU A | 252 | | 908 | | 123.227 | 1.00 23.52 |
| ATOM | 2005 | CA | LEU A | 252 | 41 | L.806 | 14.117 | 122.919 | 1.00 26.53 |
| ATOM | 2006 | CB | LEU A | 252 | 41 | 057 | 12.930 | 122.293 | 1.00 25.74 |
| | 2007 | ÇG | LEU A | | | .266 | 12.001 | 123.221 | 1.00 28.49 |
| MOTA | 2008 | | LEU A | | | .122 | 12.753 | 123.868 | 1.00 27.67 |
| ATOM | 2009 | | LEU A | | | 727 | 10.835 | 122.414 | 1.00 32.00 |
| MOTA | | | LEU A | | | 2.842 | 14 638 | 121.932 | 1.00 27.53 |
| MOTA | 2010 | C | | | | 2.528 | | 121.055 | 1.00 24.42 |
| ATOM | 2011 | 0 | LEU A | | | | 11.999 | 122.078 | 1.00 24.60 |
| ATOM | 2012 | N | LEU A | | | 1.075 | 14.170 | 121.204 | 1.00 25.04 |
| MOTA | 2013 | CA | LEU A | | | 5.157 | | | 1.00 22.48 |
| ATOM | 2014 | CB | LEU A | | | 5.176 | | 122.017 | 1.00 22.45 |
| ATOM | 2015 | CG | LEU A | | | 7.456 | 15.880 | 121.323 | |
| ATOM | 2016 | | LEU A | | | 7.105 | 16.833 | 120.175 | 1.00 23.05 |
| ATOM | 2017 | CD2 | LEU A | 253 | 48 | 3.348 | 16.578 | 122.360 | 1.00 16.40 |
| ATOM | 2018 | С | LEU A | 253 | 45 | 5.822 | 13.374 | 120.580 | 1.00 23.55 |
| ATOM | 2019 | 0 | LEU A | 253 | 46 | 5.329 | 12.516 | 121.303 | 1.00 22.11 |
| ATOM | 2020 | N | GLN A | 254 | 45 | 5.811 | 13.287 | 119.248 | 1.00 22.33 |
| ATOM | 2021 | CA | GLN A | 254 | 46 | 5.417 | 12.150 | 118.552 | 1.00 19.84 |
| ATOM | 2022 | CB | GLN A | | 45 | 5.542 | 11.731 | 117.348 | 1.00 23.09 |
| | 2023 | CG | GLN A | | 46 | 5.075 | 12.038 | 115.963 | 1.00 35.49 |
| MOTA | 2024 | CD | GLN A | | | 7.073 | 11.017 | 115.453 | 1.00 31.26 |
| ATOM | | OE1 | GLN A | | | 5.712 | 9.937 | 114.961 | 1.00 33.69 |
| ATOM | 2025 | | GLN A | | | 3.338 | 11 349 | 115.574 | 1.00 31.02 |
| : TOM | 2026 | NE2 | | | | 7.831 | 12 576 | 118.153 | 1.00 22.46 |
| TOM | 2027 | C | GLN A | | | | 12.570 | 117.478 | 1.00 17.56 |
| rom | 2028 | 0 | GLN A | | | 3.034 | 13.333 | 118.590 | 1.00 17.64 |
| ATOM | 2029 | N | LEU A | | | 3.804 | 11./01 | 118.383 | 1.00 17.04 |
| MOTA | 2030 | CA | LEU A | 255 | | 213 | | | 1.00 14.75 |
| ATOM | 2031 | CB | LEU A | 255 | | 0.894 | 12.136 | 119.750 | |
| ATOM | 2032 | CG | LEU A | 255 | | 277 | 13.196 | 120.670 | 1.00 25.02 |
| ATOM | 2033 | CD1 | LEU A | 255 | 50 | 732 | 12.996 | 122.107 | 1.00 21.99 |
| ATOM | 2034 | CD2 | LEU A | 255 | 50 | 0.636 | 14.578 | 120.149 | 1.00 18.30 |
| MOTA | 2035 | С | LEU A | 255 | 51 | 1.023 | 11.169 | 117.476 | 1.00 21.34 |
| | 2036 | ō | LEU A | | | 2.089 | 10.705 | 117.875 | 1.00 18.73 |
| ATOM | 2037 | N | GLY A | | | 0.543 | 10.928 | 116.259 | 1.00 22.75 |
| ATOM | | CA | GLY A | 256 | | 1.291 | 10.093 | 115.330 | 1.00 24.09 |
| MOTA | 2038 | | GLY. A | | | 2.660 | 10.721 | 115.126 | 1.00 24.27 |
| ATOM | 2039 | C | GLY A | 256 | | 2.805 | 11 945 | 115.134 | 1.00 19.15 |
| MOTA | 2040 | 0 | THR A | 250 | | 3.680 | 77.242 | 114.948 | 1.00 24.14 |
| ATOM | 2041 | N | THE Y | 257 | | 5.014 | 10 440 | 114.765 | 1.00 21.32 |
| MOTA | 2042 | CA | THR A | 43/ 257 | _ | | 10.440 | 115.511 | 1.00 17.24 |
| MOTA | 2043 | CB | THR A | 23/ | | 5.048 | 9.582 | 115.004 | 1.00 17.48 |
| ATOM | 2044 | 0G1 | THR A | 257 | | 5.009 | 8.248 | 117 014 | 1.00 17.30 |
| ATOM | 2045 | CG2 | THR A | 257 | | 5.728 | | 117.016 | 1.00 22.98 |
| ATOM | 2046 | C | THR A | 257 | 5 | 5.403 | 10.527 | 113.290 | 1.00 22.30 |

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|--------------|------------------------------|----------------|------------------|------------------------|--------------------|------------------|-------|
| OTA | 4 2047 O T | HR A 257 | 56.51 | 7 10 041 | 112 02. | | |
| 1OTA | 1 2048 N A | SP A 258 | 54.49 | | 112.974 | 1.00 | 20.39 |
| ATON | 1 2049 CA AS | SP A 258 | 54.86 | | 112.379 | | 22.20 |
| ATOM | 1 2050 CB AS | SP A 258 | 53.84 | | 110.961 110.056 | 1.00 | |
| MOTA | 1 2051 CG AS | SP A 258 | 52.41 | | 110.056 | | 25.06 |
| ATOM | 1 2052 C AS | SP A 258 | 55.22 | 11.596 | 110.252 | 1.00 | |
| MOTA | I 2053 O AS | SP A 258 | 55.75 | 11.390 | 110.364 | 1.00 | 27.87 |
| ATOM | 2054 OD1 AS | SP A 258 | 52.173 | | | 1.00 | 25.61 |
| ATOM | 2055 OD2 AS | P A 258 | 51.513 | | 110.742 | 1.00 | 29.86 |
| ATOM | 2056 N PR | O A 259 | 54.884 | | 109.869 | 1.00 | 33.25 |
| ATOM | 2057 CD PR | O A 259 | 54.019 | | 111.045 | 1.00 | 31.06 |
| ATOM | 2058 CA PR | O A 259 | 55.268 | | 112.220 | 1.00 | 28.59 |
| MOTA . | 2059 CB PR | O A 259 | 54.447 | | 110.469 11.296 | 1.00 | 30.95 |
| ATOM | | O A 259 | 54.418 | | 12.636 | 1.00 | 35.06 |
| MOTA | 2061 C PR | O A 259 | 56.790 | | 10.583 | 1.00 | 35.26 |
| MOTA | 2062 O PR | O A 259 | 57.300 | | 10.044 | 1.00 | 29.06 |
| MOTA | 2063 N LE | U A 260 | 57.508 | | 11.280 | 1.00 | 29.70 |
| MOTA | 2064 CA LE | U A 260 | 58.960 | | 11.455 | 1.00 | 22.68 |
| MOTA | 2065 CB LET | J A 260 | 59.461 | 12.576 1 | 12 533 | 1.00 2 | 28.41 |
| ATOM | 2066 CG LET | J A 260 | 58.970 | | 13.969 | 1.00 2 | 22.47 |
| ATOM | 2067 CD1 LET | J A 260 | 59.352 | 11.599 1 | 14 826 | 1.00 2 | 20.14 |
| MOTA | 2068 CD2 LEU | J A 260 | 59.592 | 14.079 1 | | 1.00 2 | 22.83 |
| MOTA | 2069 C LEU | | 59.770 | 13.344 1 | | 1.00 2 | 20.48 |
| ATOM | 2070 O LEU | J A 260 | 59.407 | 12.535 1 | | 1.00 2 | 7 02 |
| MOTA | 2071 N LEU | A 261 | 60.874 | 14.081 1 | | 1.00 2 | 67.03 |
| ATOM | 2072 CA LEU | A 261 | 61.742 | 14.010 10 | 08.865 | 1.00 2 | 6 56 |
| MOTA MOTA | 2073 CB LEU 2074 CG LEU | A 261 | 63.067 | 14.737 10 | 09.137 | 1.00 2 | 3 06 |
| ATOM | | A 261 | 64.131 | 14.615 10 | | 1.00 2 | 9.52 |
| MOTA | | A 261 A 261 | 63.642 | 15.325 10 | 06.770 T | 1.00 2 | 2.68 |
| ATOM | 2077 C LEU | A 261 A 261 | 65.460 | 15.219 10 | 08.475 | 1.00 2 | 6.71 |
| MOTA | | A 261 | 62.063 | | 08.443 | 1.00 2 | 8.23 |
| ATOM | 2079 N GLU | A 262 | 61.880 | 12.198 10 | 7.289 | 1.00 2 | 6.52 |
| ATOM | | A 262 | 62.539 62.938 | 11.787.10 | | 1.00 2 | 8.70 |
| ATOM | 2081 CB GLU | A 262 | 63.685 | 10.416 10 | | L.00 3. | 1.76 |
| ATOM | | A 262 | 64.890 | 9.855 11 10.683 11 | 0.351 | 1.00 2 | 9.72 |
| ATOM | | A 262 | 64.521 | 11.847 11 | 0.803 1 | 1.00 3 | 1.33 |
| MOTA | 2084 OE1 GLU | A 262 | 63.324 | 12.195 11 | | 1.00 28 | |
| ATOM | 2085 OE2 GLU | A 262 | 65.433 | 12.424 11 | | 00 28 | 8.75 |
| ATOM | 2086 C GLU | A 262 | 61.847 | | | 00 26 | 2.08 |
| ATOM | 2087 O GLU | A 262 | 62.158 | | | .00 28 | 3.63 |
| ATOM | 2088 N ASP | A 263 . | 60.582 | | | .00 28 | 7.72 |
| ATOM | 2089 CA ASP | A 263 | 59.513 | | | .00 26 | .07 |
| ATOM | | A 263 | 58.305 | | | .00 25 | |
| ATOM ATOM | 2091 CG ASP 2092 OD1 ASP | A 263 | 57.261 | 7.998 109 | | .00 33 | . 14 |
| ATOM | | A 263 | 56.638 | 7.636 110 | | .00 29 | . 91 |
| ATOM | | A 263 | 57.042 | 7.509 108 | 3.051 1 | .00 26 | .56 |
| ATOM | 2094 C ASP 2 2095 O ASP 2 | 4 403 | 59.150 | 9.146 106 | 5.957 1 | .00 29 | .44 |
| ATOM | 2096 N TYR | 1 203 | 58.740 | 10.247 106 | 5.594 1 | .00 24 | .70 |
| ATOM | 2097 CA TYR A | 204 | 59.303 | 8.111 106 | | .00 27 | .51 |
| MOTA | 2098 CB TYR A | 264 | 59.031 59.576 | 8.219 104 | | .00 33 | . 89 |
| MOTA | 2099 CG TYR A | | 61.059 | 7.008 103 | | 00 40 | . 44 |
| MOTA | 2100 CD1 TYR A | 264 | 61.565 | 6.771 104 | | 00 50 | . 64 |
| MOTA | 2101 CE1 TYR A | 264 | 62.933 | 6.087 105 | | 00 54 | . 67 |
| MOTA | 2102 CD2 TYR A | 264 | 61.960 | 5.876 105 | | 00 55 | . 28 |
| | 2103 CE2 TYR A | | 63.329 | 7.242 103 7.038 103 | | 00 53 | . 79 |
| | 2104 CZ TYR A | | 63.809 | 6.354 104 | | 00 56 | |
| | 2105 OH TYR A | | 65.161 | 6.147 104 | | 00 56. | |
| | 2106 C TYR A | 264 | 57.561 | 8.394 104 | | 00 55. 00 31. | 30 |
| | 2107 O TYR A | | 57.311 | 8.825 103 | | 00 31. | 15 |
| | 2106 N LEU A | | 56.641 | 8.059 105 | | 00 27. | |
| | 2109 CA LEU A | | 55.244 | 8.209 104 | | 00 24. | |
| | 2110 CB LEU A | | 54.360 | 7.189 105 | | 00 24. 00 26. | |
| | 2111 CG LEU A | | 54.663 | 5.724 105 | | 00 29. | |
| TOM : | 2112 CD1 LEU A | 265 | 53.464 | 4.836 105 | | 00 21. | 17 |
| | | | | | | • | |

| ATOM | 2113 | CD2 | LEU A | 265 | | 54.931 | 5.620 | 103.682 | 1.00 | 33.35 |
|--------------|--------------|--------|----------------|-----|---|------------------|------------------|--------------------|------|----------------|
| ATOM | 2114 | C | LEU A | | | 54.669 | 9.617 | | | 20.81 |
| ATOM | 2115 | ō | LEU A | | | 53.457 | 9.796 | | | 21.30 |
| ATOM | 2116 | N | SER A | | | 55.540 | 10.622 | 104.959 | | 23.23 |
| ATOM | 2117 | CA | SER A | | | 55.084 | 12.011 | | | 26.30 |
| ATOM | 2118 | CB | SER A | | | 54.856 | 12.502 | 106.444 | | 25.16 |
| ATOM | 2119 | OG | SER A | | | 56.074 | 12.845 | 107.084 | | 22.92 |
| ATOM | 2120 | c | SER A | | | 56.147 | 12.879 | | | 30.17 |
| ATOM | 2121 | ō | SER A | | | 57.334 | 12.555 | | | 31.65 |
| ATOM | 2122 | N | LYS A | | | 55.731 | 13.985 | | | 31.56 |
| ATOM | 2123 | CA | LYS A | | | 56.696 | 14.873 | 103.140 | | 27.65 |
| ATOM | 2124 | CB | LYS A | | | 56.140 | 15.425 | 101.834 | | 30.54 |
| ATOM | 2125 | CG | LYS A | | | 55.815 | 14.327 | 100.819 | | 34.13 |
| ATOM | 2126 | CD | LYS A | | | | 13.463 | 100.549 | 1.00 | 29.09 |
| ATOM | 2127 | CE | LYS A | | | 56.745 | 12.376 | 99.524 | 1.00 | 37.61 |
| ATOM | 2128 | NZ | LYS A | | | 57.956 | 11.541 | 99.272 | | 31.91 |
| ATOM | 2129 | С | LYS A | | | 57.050 | 16.004 | 104.107 | 1.00 | 30.85 |
| ATOM | 2130 | 0 | LYS A | | • | 57.624 | 17.017 | 103.707 | 1.00 | 27.86 |
| ATOM | 2131 | N | PHE A | 268 | | 56.688 | 15.826 | 105.377 | 1.00 | 24.19 |
| ATOM | 2132 | CA | PHE A | 268 | | 57.009 | 16.808 | 106.412 | 1.00 | 25.34 |
| ATOM | 2133 | CB | PHE A | 268 | | 56.014 | 16.730 | 107.579 | 1.00 | 24.54 |
| ATOM | 2134 | CG | PHE A | 268 | | 54.636 | 17.256 | 107.257 | 1.00 | 21.68 |
| ATOM | 2135 | CD1 | PHE A | 268 | | 53.631 | 17.221 | 108.216 | 1.00 | 28.65 |
| ATOM | 2136 | CD2 | PHE A | 268 | | 54.346 | 17.806 | | | 25.14 |
| ATOM | 2137 | CE1 | PHE A | | | 52.357 | 17.728 | 107.944 | | 25.34 |
| ATOM | 2138 | CE2 | PHE A | 268 | | 53.077 | 18.315 | 105.730 | | 23.79 |
| MOTA | 2139 | CZ | PHE A | | | 52.082 | 18.275 | 106.702 | | 28.13 |
| MOTA | 2140 | С | PHE A | | | 58.410 | 16.470 | 106.908 | | 25.66 |
| MOTA | 2141 | 0 | PHE A | | | 58.778 | 15.299 | 106.994 | | 28.44 |
| ATOM | 2142 | N | ASN A | | | 59.194 | 17.490 | | | 25.81 |
| ATOM | 2143 | CA | ASN A | | | 60.555 | 17.270 | | | 30.60 |
| ATOM | 2144 | CB | ASN A | | | 61.566 | 17.938 | 106.767 | | 31.97 |
| MOTA | 2145 | CG | ASN A | | | 61.392 | 17.513 | 105.317 | | 35.83 33.93 |
| MOTA | 2146 | OD1 | ASN A | | | 61.235 | 16.332 18.477 | 105.020 104.405 | | 33.95 |
| MOTA | 2147 | ND2 | ASN A | | | 61.446 60.723 | 17.843 | 109.110 | | 31.80 |
| ATOM | 2148 | C O | ASN A | | | 61.609 | 18.665 | 109.110 | | 28.13 |
| MOTA | 2149 | Ŋ | LEU A | | | 59.888 | 17.397 | 110.043 | | 29.70 |
| ATOM | 2150 2151 | CA | LEU A | | | 59.954 | 17.918 | 111.406 | | 26.87 |
| ATOM ATOM | 2152 | CB | | 270 | | 58.575 | 17.833 | 112.074 | | 26.60 |
| ATOM | 2153 | CG | LEU A | | | 57.392 | 18.425 | 111.297 | | 29.62 |
| ATOM | 2154 | CD1 | LEU A | | | 56.177 | 18.494 | 112.222 | | 28.54 |
| ATOM | 2155 | CD2 | LEU A | | | 57.740 | 19.825 | 110.790 | 1.00 | 29.40 |
| ATOM | 2156 | C | LEU A | | | 60.979 | 17.242 | 112.301 | 1.00 | 26.83 |
| ATOM | 2157 | 0 | LEU A | 270 | | 61.490 | 16.158 | 111.990 | 1.00 | 19.60 |
| MOTA | 2158 | N | SER A | 271 | | 61.275 | 17.896 | 113.420 | | 21.66 |
| ATOM | 2159 | CA | SER A | 271 | | 62.220 | 17.365 | 114.393 | | 27.08 |
| MOTA | 2160 | CB | SER A | 271 | | 63.189 | 18.460 | 114.846 | | 24.64 |
| ATOM | 2161 | OG | SER A | | | 62.499 | 19.433 | 115.626 | | 18.60 |
| ATOM | 2162 | С | SER A | 271 | | 61.454 | 16.868 | 115.618 | | 23.70 |
| MOTA | 2163 | 0 | SER A | | | 60.272 | 17.150 | 115.772 | 1.00 | 22.56 |
| MOTA | 2164 | | ASN A | | | 62.157 | 16.129 | 116.470 | | 28.35 |
| MOTA | 2165 | | ASN A | | | 61.649 | | 117.739 | | 31.03 |
| MOTA | 2166 | | ASN A | | | 62.774 | | 118.498 | | 28.80 |
| MOTA | 2167 | | ASN A | | | 62.854 | 13.428 | 118.180 | | 36.65 |
| MOTA | 2168 | | ASN A | | | 63.712 | 12.709 | 118.705 | | 29.89 |
| MOTA | 2169 | | ASN A | | | 61.953 | | 117.319 | | 40.80 |
| MOTA | 2170 | | ASN A | | | 61.167 | | 118.661 119.261 | | 27.50 |
| ATOM | 2171 | | ASN A. | | | 60.090 | 17 603 | 119.261 | | 31.49 |
| ATOM | 2172 | | VAL A VAL A | | | 62.032 | 10.075 | 119.667 | | 31.58 |
| ATOM | 2173 | | VAL A | | | 61.802 63.069 | 10.53/ | 119.725 | | 35.80 |
| ATOM | 2174 2175 | | VAL A | | | 62.804 | 20 000 | 120.500 | | 48.07 |
| ATOM | | CGI | VAL A | 273 | | 64.198 | | 120.381 | | 42.81 |
| ATOM | 2176 2177 | | VAL A | | | 60.608 | 19 665 | 119.234 | 1.00 | 30.13 |
| ATCM | 2178 | | VAL A | | | 59.872 | 20.174 | 120.072 | 1.00 | 31.44 |
| atom | 2110 | • | ****** | • | | | 50.1.2 | | | _ |

| | | • |
|-------|---------------------|---|
| ATO. | M 2179 N ALA A 274 | 60.405 19.800 117 929 1 00 24 1 |
| ATO | M 2180 CA ALA A 274 | |
| ATOI | | 33.238 20.558 117.455 1.00 26 2° |
| ATO | 11 2/4 | 33.341 20.780 115.965 1.00 21 ac |
| ATO | C ALLA X Z/4 | 58.005 19.759 117 789 1 00 25 66 |
| ATON | NUA A 2/4 | |
| | | 50 100 25.76 |
| ATON | 1 2185 CA PHE A 275 | E7 01 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 |
| ATOM | 1 2186 CB PHE A 275 | 57 440 23.89 |
| ATOM | 1 2187 CG PHE A 275 | EC 3.6 |
| ATOM | | 30.340 15.088 117.870 1.00 28 9E |
| ATOM | | 55.278 15.064 116.982 1.00 32 60 |
| ATOM | EDE FILE A 2/3 | 56.365 14.166 118.910 1 00 29 02 |
| ATOM | 422 IIIE A 2/3 | 54.248 14.132 117 119 1 00 33 77 |
| ATOM | | |
| | co tue w 7/2 | E4 200 10 10 10 10 10 10 10 10 10 10 10 10 1 |
| ATOM | - III R 2/3 | 55 500 |
| MOTA | 2194 O PHE A 275 | EE 400 40 123 1.00 24.03 |
| ATOM | 2195 N LEU A 276 | |
| ATOM | 2196 CA LEU A 276 | 3/.534 1/.6/3 120.331 1.00 25 45 |
| ATOM | | 37.337 17.837 121.766 1.00 27 94 |
| ATOM | | 58.667 17.692 122.534 1 00 25 11 |
| ATOM | DEO M 2/0 | 58.651 18.132 124 001 1 00 31 15 |
| | 2199 CD1 LEU A 276 | 57.609 17.351 124 761 1 00 31.13 |
| ATOM | 2200 CD2 LEU A 276 | 60 033 10 1.00 29.37 |
| ATOM | 2201 C LEU A 276 | EC 350 1 1.00 2/.30 |
| ATOM | 2202 O LEU A 276 | EE 050 10 10 10 10 10 10 10 10 10 10 10 10 10 |
| ATOM | 2203 N LYS A 277 | E7 757 65 1-0 1-0 20.09 |
| MOTA | 2204 CA LYS A 277 | 56.333. 20.219 121.425 1.00 30.99 |
| ATOM | 2205 CB LYS A 277 | 30.913 21.593 121.603 1.00 27 04 |
| ATOM | 2206 CG LYS A 277 | 3/-/42 22-516 120,704 1,00 30 30 |
| ATOM | 220 11 2// | 57.941 23.934 121.237 1.00 36 46 |
| ATOM | 11 4// | 56.633 24.668 121 454 1 00 42 22 |
| ATOM | A 2 // | 56.870 26.059 122.049 1 00 45 70 |
| ATOM | | 57.528 26.004 123 390 1 00 44 64 |
| | 2210 C LYS A 277 | EE 430 m 1.00 44.04 |
| ATOM | 2211 O LYS A 277 | E4 C40 30.20 |
| ATOM | 2212 N ALA A 278 | EF 05- |
| ATOM | 2213 CA ALA A 278 | E |
| ATOM | 2214 CB ALA A 278 | E2 100 223.070 1.00 30.31 |
| ATOM | 2215 C ALA A 278 | E2 200 00 1100 20.30 |
| ATOM | 2216 O ALA A 278 | 32.789 20.527 120.786 1.00 30 99 |
| ATOM | 2217 N PHE A 279 | 31.735 21.067 121.108 1.00 30 36 |
| ATOM | 2218 CA PHE A 279 | 33.245 19.422 121.360 1.00 27 85 |
| ATOM | 112 11 2/3 | 52.540 18.759 122.448 1.00 29 62 |
| ATOM | | 53.343 17.534 122.886 1.00 26 83 |
| ATOM | | 52.786 16.823 124.078 1.00 29.11 |
| | | 51.556 16.176 124 015 1 00 20 06 |
| ATOM | 2222 CD2 PHE A 279 | |
| MOTA | 2223 CE1 PHE A 279 | E1 A=4 |
| MOTA | 2224 CE2 PHE A 279 | E2 000 27.30 |
| ATOM | 2225 CZ PHE A 279 | E3 30. 1.00 38.(I) |
| ATOM | 2226 C PHE A 279 | |
| ATOM | 2227 O PHE A 279 | C1 D2= |
| ATOM | 2228 N ASN A 280 | 53 |
| ATOM | 2229 CA ASN A 280 | 53.432 20.429 123.990 1.00 32.03 |
| ATOM | 2230 CB ASN A 280 | 23.339 21.373 125.104 1.00 30 54 |
| | - 11011 11 200 | 34.724 21.819 125.583 1.00 26 79 |
| ATOM | | 55.508 20.695 126.227 1.00 33.68 |
| | | |
| MOTA | 2233 ND2 ASN A 280 | |
| MOTA | 2234 C ASN A 280 | 53 403 1100 200.073 1.00 33.59 |
| MOTA | 2235 O ASN A 280 | E1 000 00 10 10 10 10 10 10 10 10 10 10 1 |
| | 2236 N ILE A 281 | E3 420 27.00 |
| MOTA | 2237 CA ILE A 281 | E1 630 01 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 |
| MOTA | 2238 CB ILE A 281 | 51 070 01-01 223 220 1.00 31.07 |
| | 2239 CG2 ILE A 281 | 51.878 24.517 121.666 1.00 35.08 |
| | 2240 CG1 ILE A 281 | 30.776 25.445 121.174 1.00 34 33 |
| | | 53.253 25.185 121.562 1.00 33.53 |
| | | 53.590 25.694 120 178 1 00 34 00 |
| | 2242 C ILE A 281 | 50.141 23.798 123.329 1 00 31 22 |
| | 2243 O ILE A 281 | 40 301 |
| TOM 2 | 2244 N VAL A 282 | 40 700 |
| | | 49.723 22.606 122.923 1.00 30.91 |
| | | |

```
22.214 123.081
                                                            1.00 30.76
                                   48.332
MOTA
        2245
               CA
                   VAL A 282
                                                                  35.10
                                            20.797 122.523
                                                             1.00
                                   48.075
                   YAL A 282
        2246
               CB
MOTA
                                                             1.00 28.72
               CG1 VAL A 282
                                   46.641
                                            20.358 122.841
ATOM
        2247
                                            20:781 121.018
                                                             1.00 28.66
                                   48.313
        2248
               CG2
                   VAL A 282
MOTA
                                            22.236 124.558
                                                             1.00 31.39
                                   47.952
                   VAL A 282
        2249
               C
ATOM
                                                             1.00 32.70
                                            22.715
                                                   124.917
                                   46.884
                   VAL A 282
        2250
               0
ATOM
                                                             1.00 29.86
                                            21.720 125.406
                   ARG A 283
                                   48.837
        2251
               N
MOTA
                                            21.675 126.840
                                                             1.00 34.82
                                   48.587
                   ARG A 283
MOTA
        2252
               CA
                                                             1.00 31.44
                                            20.785
                                                   127.519
                                   49.629
        2253
               CB
                   ARG .A 283
ATOM
                                                              1.00 29.49
                                            19.334 127.061
                                   49.551
                   ARG A 283
        2254
               CG-
MOTA
                                            18.539 127.554
                                                             1.00 30:67
                   ARG A 283
                                   50.729
MOTA
        2255
               CD
                                                              1.00 30.78
                                            18.314 128.990
                                   50.730
        2256
               NE
                   ARG . A 283
MOTA
                                                              1.00 35.27
                                            18.351 129.742
                   ARG A 283
                                   51.826
        2257
               CZ
MOTA
                                                              1.00 36.46
                                            18.611 129.198
                   ARG A 283
                                    53.012
MOTA
        2258
               NH1
                                                              1.00 35.90
                                    51.742
                                            18.100 131.035
        2259
                   ARG A 283
               NH2
MOTA
                                    48.561
                                            23.065 127.473
                                                              1.00 36.06
                   ARG A 283
               C
        2260
 MOTA
                                            23.302 128.439
                                                              1.00 35.04
                                    47.830
                   ARG A 283
 MOTA
        2261
               0
                                                              1.00 35.70
                                    49.350
                                            23.985 126.928
                   GLU A 284
               N
        2262
ATOM
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               CA
                   GLU A 284
        2263
 MOTA
                                                              1.00 44.17
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                   GLU A 284
                                    50.499
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               CB
 MOTA
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                   GLU A 284
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        2265
               CG
 MOTA
                                                              1.00 60.69
                                            26.495 126.401
                                    52.989
               CD
                   GLU A 284
        2266
 ATOM
                                            27.738 126.542
                                                              1.00 63.13
                                    53.012
                   GLU A 284
               OE1
 ATOM
        2267
                                            25.880 125.680
                                                              1.00 62.79
                   GLU A 284
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        2268
               OE<sub>2</sub>
 ATOM
                                                              1.00 39.24
                                            26.014 127.148
                                    48.039
                    GLU A 284
 MOTA
        2269
                                            26.783 127.954
                                                              1.00 38.52
                                    47.525
                   GLU A 284
        2270
 ATOM
                                                              1.00 33.75
                                            25.704 125.986
                                    47.472
                   VAL A 285
        2271
               N
 MOTA
                                            26.294 125.592
                                                              1.00 35.82
                                    46.205
                   VAL A 285
         2272
               CA
 ATOM
                                                              1.00 34.14
                                            26.291 124.062
                                    46.039
                    VAL A 285
        2273
               CB
 MOTA
                                            26.811 123.693
                                                              1.00 36.43
                                    44.654
                   VAL A 285
               CG1
        2274
 MOTA
                                            27.153 123.419
                                                              1.00 37.26
                   VAL A 285
                                    47.114
        2275
               CG2
 ATOM
                                                              1.00 38.96
                                             25.638 126.192
                                    44.964
                    VAL A 285
         2276
               С
 ATOM
                                                              1.00 41.83
                                            26.336 126.611
                                    44.043
         2277
               O
                    VAL A 285
 ATOM
                                    44.931
43.760
                                             24.308 126.236
                                                              1.00 37.57
                    PHE A 286
         2278
               N
 MOTA
                                             23.608 126.753
                                                              1.00 35.05
                    PHE A 286
         2279
               CA
 MOTA
                                                              1.00 32.53
                                             22.723 125.657
                                    43.159
 ATOM
         2280
               CB
                    PHE A 286
                                                              1.00 30.15
                                    42.544
                                             23.490 124.529
                    PHE A 286
         2281
               CG
 ATOM
                                             23.459 123.256
                                                              1.00 33.96
                                    43.104
               CD1
                    PHE A 286
         2282
 ATOM
                                                              1.00 30.30
                                             24.245 124.736
                   PHE A 286
                                    41.398
         2283
               CD2
 ATOM
                                                              1.00 32.96
                                             24.170 122.202
                                    42.527
                    PHE A 286
         2284
               CE1
 MOTA
                                             24.958 123.693
                                                              1.00 31.67
                                    40.813
               CE2
                    PHE A 286
         2285
 MOTA
                                                              1.00 31.66
                                             24.919
                                                    122.419
                    PHE A 286
                                    41.381
         2286
               CZ
 ATOM
                                                              1.00 35.18
                                    43.922
                                             22.773
                                                    128.015
                    PHE A 286
         2287
               C
 MOTA
                                                              1.00 36.97
                                             22.080 128.409
                                    42.984
         2288
               0
                    PHE A 286
 ATOM
                                    45.086
                                             22.840 128.656
                                                              1.00 30.87
                    GLY A 287
 ATOM
         2289
               N
                                                              1.00 30.06
                                             22.056 129.862
                                    45.297
                    GLY 2 287
 ATOM
         2290
               CA
                                                               1.00 34.44
                                    45.525
                                             20.590 129.527
         2291
               C-
                    GLY 1. 287
 MOTA
                                    45.914
                                                              1.00 32.54
                                             20.264 128.403
                    GLY 7. 287
               О
         2292
 MOTA
                                                              1.00 28.42
                                             19.710 130.500
                    GLU A 288
                                    45.288
 MOTA
         2293
               N
                                                               1.00 32.23
                                             18.273 130.310
                                    45.464
                    GLU A 288
         2294
               CA
 ATOM
                                                               1.00 37.02
                                    45.613
                                             17.576
                                                    131.663
                    GLU A 288
         2295
               CB
 ATOM
                                                               1.00 45.36
                                             17.864 132.411
                                    46.910
                    GLU A 288
 ATOM
         2296
               CG
                                                               1.00 45.65
                                             17.455 131.622
                                    48.140
                    GLU A 288
         2297
               CD
 ATOM
                                                               1.00 46.42
                                             16.334
                                                     131.069
                                    48.144
                    GLU A 288
         2298
               OE1
 MOTA
                                                               1.00 50.78
                                             18.245 131.571
                                    49.106
                   GLU A 288
         2299
 MOTA
               OE2
                                                               1.00 30.98
                                             17.623 129.546
                                    44.309
                    GLU A 288
         2300
               C
 MOTA
                                                               1.00 28.67
                                             17.957 129.762
                                    43.144
         2301
               O
                    GLU A 288
 ATOM
                                                               1.00 29.66
                                             16.694 128.657
                                    44.641
                    GLY A 289
         2302
               N
 MOTA
                                                               1.00 28.08
                                                     127.886
                                             15.999
                    GLY A 289
                                    43.625
         2303
               CA
 MOTA
                                                               1.00 30.45
                                                     127.861
                                    43.922
                                             14.510
                    GLY A 289
         2304
               C
 ATCM
                                                               1.00 25.90
                                    44.618
                                             14.307 128.739
                    GLY A 389
         2305
               0
 ATCM
                                             13.807 126.868
                                                               1.00 26.21
                    VAL A 290
                                    43.384
         2306
               N
  ATOM
                                                               1.00 27.31
                                             12.373 126.718
                                    43.612
                    VAL A 290
         2307
               CA
  MOTA
                                                               1.00 26.53
                                             11.626 126.412
                                    42.288
                    VAL A 290
         2308
                CB
 ATOM
                                             10.148 126.204
                                                               1.00 25.36
                                    42.554
                    VAL A 290
         2309
                CG1
  ATOM
                                             11.822 127.565
                                                               1.00 24.38
                                    41.308
                    VAL A 290
                CG2
         2310
  ATOM
```

| ATO | M 2311 | C VAL A 290 | 44.58 | 0 12 248 125 55 | |
|-------------|----------|---------------|----------|-----------------|--------------|
| ATO | M 2312 | O VAL A 290 | 44.30 | | |
| ATO: | M 2313 | N TYR A 291 | | | |
| ATO | | CA TYR A 291 | 45.71 | | 1 00 23 56 |
| ATO | | CB TYR A 291 | 46.72 | | 2 1.00 23 74 |
| ATO | | | 48.092 | | 1.00 18.40 |
| ATO | , | CG TYR A 291 | 48.040 | 13.113 126.118 | 1.00 21.60 |
| | | CD1 TYR A 291 | 48.326 | 13.148 127.483 | |
| ATO | | CE1 TYR A 291 | 48.200 | | |
| ATO | - | CD2 TYR A 291 | 47.634 | | |
| ATO | - | CE2 TYR A 291 | 47.504 | 15.476 126.220 | |
| ATOM | 1 2321 | CZ TYR A 291 | 47.786 | 15.489 127.575 | |
| ATOM | 1 2322 | OH TYR A 291 | 47.631 | | |
| ATOM | 1 2323 | C TYR A 291 | | | |
| ATOM | | O TYR A 291 | 46.768 | | 1.00 23.03 |
| ATOM | | N LEU A 292 | 46.837 | | 1.00 20.66 |
| ATOM | | CA LEU A 292 | 46.755 | | 1.00 23.96 |
| ATOM | | | 46.767 | 8.924 121.902 | 1.00 20.69 |
| ATOM | | | 45.482 | 8.842 121.076 | 1.00 22.13 |
| | | CG LEU A 292 | 44.162 | 9.063 121.814 | 1.00 23.78 |
| ATOM | 2329 (| CD1 LEU A 292 | 43.001 | 8.959 120.826 | 1.00 23.78 |
| MOTA | 2330 (| CD2 LEU A 292 | 44.008 | 8.050 122.930 | 1.00 23.09 |
| ATOM | | | 47.953 | 8.885 120.947 | 1.00 16.01 |
| MOTA | 2332 (| | . 48.527 | 9.923 120.617 | 1.00 22.90 |
| ATOM | 2333 N | | 48.301 | 7.923 120.617 | 1.00 22.31 |
| ATOM | 2334 (| A GLY A 293 | | 7.684 120.491 | 1.00 18.83 |
| ATOM | 2335 C | | 49.401 | 7.529 119.554 | 1.00 24.35 |
| ÀTOM | 2336 0 | | 48.908 | | 1.00 24.22 |
| ATOM | 2337 N | | 48.025 | 8.684 117.991 | 1.00 20.46 |
| ATOM | 2338 C | 7 CIV > 204 | 49.459 | 7.177 117.148 | 1.00 24.63 |
| ATOM | 2339 C | 253 | 49.035 | 7.423 115.779 | 1.00 22.03 |
| ATOM | | | 50.024 | 6.869 114.769 | 1.00 22.90 |
| | | | 50.956 | 6.150 115.136 | 1.00 24.10 |
| ATOM | 2341 N | | 49.825 | 7.203 113.499 | 1.00 19.85 |
| ATOM | 2342 C | | 50.721 | 6.724 112.458 | 1.00 23.33 |
| ATOM | 2343 C | GLY A 295 | 52.185 | 7.010 112.740 | 1.00 19.01 |
| ATOM | 2344 0 | GLY A 295 . | 52.541 | 8.094 113.196 | 1.00 19.01 |
| ATOM | 2345 N | GLY A 296 | 53.035 | 6.026 112.472 | 1.00 19.39 |
| ATOM | 2346 C | | 54.468 | 6.162 112.690 | 1.00 25.85 |
| ATOM | 2347 C | GLY A 296 | 55.098 | 4.898 112.146 | 1.00 22.65 |
| ATOM | 2348 O | GLY A 296 | 54.778 | 3.798 112.609 | 1.00 25.31 |
| ATOM | 2349 N | TYR A 297 | 56.005 | | 1.00 25.86 |
| ATOM | 2350 CA | | 56.598 | 5.034 111.185 | 1.00 22.83 |
| ATOM | 2351 CB | | | 3.852 110.577 | 1.00 23.93 |
| ATOM | 2352 CG | | 56.137 | 3.780 109.125 | 1.00 21.59 |
| ATOM | 2353 CD | | 54.660 | 4.084 109.035 | 1.00 25.85 |
| ATOM | 2354 CE | | 54.203 | 5.402 109.017 | 1.00 22.28 |
| ATOM | 2355 CD | | 52.842 | 5.695 109.089 | 1.00 20.19 |
| ATOM | 2356 CE | | 53.713 | 3.062 109.116 | 1.00 25.28 |
| ATOM | | | 52.352 | 3.346 109.190 | 1.00 21.83 |
| | | TYR A 297 | 51.927 | 4.666 109.181 | 1.00 21.81 |
| ATOM | 2358 ОН | TYR A 297 | 50.588 | 4.972 109.305 | 1.00 19.51 |
| ATOM | 2359 C | TYR A 297 | 58.104 | _ | 1.00 23.78 |
| TOM | 2360 o | TYR A 297 | 58.665 | | 1.00 22.07 |
| -TOM | 2361 N | HIS A 298 | 58.765 | | |
| -TOM | 2362 CA | HIS A 298 | 60.204 | | 1.00 23.71 |
| MOT. | 2363 CB | HIS A 298 | 60.913 | | 1.00 26.33 |
| ATOM | 2364 CG | HIS A 298 | 62.403 | | 1.00 28.74 |
| MOTA | | HIS A 298 | | 5.727 111.213 | 1.00 33.08 |
| TOM | 2366 ND1 | HIS A 298 | 63.273 | 5.465 112.215 | 1.00 31.83 |
| TOM | | HIS A 298 | 63.151 | 5.775 110.056 | 1.00 32.49 |
| TCM | 2368 NE2 | NIS A 256 | 64.419 | .5.547 110.345 | 1.00 29.10 |
| | | HIS A 298 | 64.520 | 5.354 111.648 | 1.00 38.70 |
| TOM | | HIS A 298 | 60.371 | 4.188 112.996 | 1.00 27.81 |
| TOM | 2370 O | HIS A 298 | 60.120 | | 1.00 25.07 |
| TOM | 2371 N | PRO A 299 | 60.829 | | .00 29.37 |
| TOM | 2372 CD | PRO A 299 | 61.285 | _ | 00 26.09 |
| TOM | 2373 CA | PRO A 299 | 61.024 | | 00 20 45 |
| TOM: | 2374 CB | PRO A 299 | 61.675 | | .00 29.46 |
| TOM | 2375 CG | PRO A 299 | 62.411 | | .00 29.03 |
| TOM | 2376 C | PRO A 299 | 61.849 | | .00 27.34 |
| | | - | | 2.403 TT3.3/0 I | .00 31.88 |
| | | | | | |

Figure 18-37

| ATOM | 2377 | 0 | PRO A | 299 | 61.480 | | 116.724 | 1.00 32.45 |
|------|------|-----|-------|-----|---------|--------|---------|------------|
| MOTA | 2378 | N | TYR A | 300 | 62.959 | .3.932 | 115.058 | 1.00 27.41 |
| MOTA | 2379 | CA | TYR A | 300 | 63.803 | 4.801 | 115.878 | 1.00 27.34 |
| ATOM | 2380 | CB | TYR A | | 65.163 | | 115.207 | 1.00 26.84 |
| | 2381 | CG | TYR A | | 65.912 | | 114.738 | 1.00 29.09 |
| ATOM | | | | | | | | |
| MOTA | 2382 | | TYR A | | 65.517 | | 115.120 | 1.00 30.93 |
| ATOM | 2383 | CE1 | TYR A | 300 | 66.214 | | 114.682 | 1.00 30.68 |
| MOTA | 2384 | CD2 | TYR A | 300 | 67.027 | 3.941 | 113.908 | 1.00 29.72 |
| ATOM | 2385 | CE2 | TYR A | 300 | 67.730 | 2.829 | 113.466 | 1.00 30.76 |
| ATOM | 2386 | CZ | TYR A | | 67.320 | 1.568 | 113.854 | 1.00 33.89 |
| | 2387 | OH | TYR A | | 68.011 | | 113.404 | 1.00 34.70 |
| ATOM | | | | | 63.113 | | 116.137 | 1.00 23.44 |
| MOTA | 2388 | C | TYR A | | | | | |
| MOTA | 2389 | 0 | TYR A | | 63.108 | | 117.264 | 1.00 23.87 |
| MOTA | 2390 | N | ALA A | | 62.530 | | 115.092 | 1.00 22.19 |
| ATOM | 2391 | CA | ALA A | _ | 61.839 | | 115.216 | 1.00 26.50 |
| MOTA | 2392 | CB | ALA A | 301 | 61.266 | 8.416 | 113.864 | 1.00 24.16 |
| ATOM | 2393 | ·c | ALA A | 301 | 60.715 | 7.878 | 116.237 | 1.00 27.86 |
| ATOM | 2394 | 0 | ALA A | | 60.556 | 8.728 | 117.117 | 1.00 22.47 |
| MOTA | 2395 | N | LEU A | | 59.940 | | 116.110 | 1.00 23.27 |
| | | | | | 58.818 | | 116.996 | 1.00 26.50 |
| ATOM | 2396 | CA | LEU A | | | | | |
| ATOM | 2397 | CB | LEU A | | 58.036 | | 116.483 | 1.00 26.02 |
| ATOM | 2398 | CG | LEU A | | 56.866 | | 117.291 | 1.00 29.73 |
| ATOM | 2399 | CD1 | LEU A | 302 | 55.983 | 3.938 | 116.394 | 1.00 31.01 |
| ATOM | 2400 | CD2 | LEU A | 302 | 57.394 | | 118.465 | 1.00 32.99 |
| ATOM | 2401 | С | LEU A | 302 | 59.246 | 6.373 | 118.451 | 1.00 27.49 |
| ATOM | 2402 | 0 | LEU A | | 58.648 | | 119.358 | 1.00 25.22 |
| ATOM | 2403 | N | ALA A | | 60.289 | | 118.672 | 1.00 27.85 |
| | 2404 | CA | ALA A | | 60.765 | | 120.024 | 1.00 27.33 |
| MOTA | | | | | 61.854 | | 119.990 | 1.00 29.17 |
| MOTA | 2405 | CB | ALA A | | | | | |
| ATOM | 2406 | С | ALA A | | 61.279 | | 120.714 | 1.00 26.64 |
| ATOM | 2407 | 0 | ALA A | | 60.944 | | 121.875 | |
| MOTA | 2408 | N | ARG A | 304 | 62.092 | | 120.003 | 1.00 27.48 |
| MOTA | 2409 | CA | ARG A | 304 | 62.648 | 8.570 | 120.581 | 1.00 25.46 |
| ATOM | 2410 | CB | ARG A | 304 | 63.773 | 9.136 | 119.704 | 1.00 21.31 |
| ATOM | 2411 | CG | ARG A | | 65.005 | 8.231 | 119.562 | 1.00 25.98 |
| | 2412 | CD | ARG A | | 66.153 | | 118.951 | 1.00 27.87 |
| MOTA | | NE | ARG A | | 65.647 | | 117.796 | 1.00 36.76 |
| MOTA | 2413 | | | | 66.207 | | 117.261 | 1.00 30.79 |
| MOTA | 2414 | CZ | ARG A | | | | | |
| MOTA | 2415 | | ARG A | | 67.323 | | 117.768 | 1.00 30.11 |
| ATOM | 2416 | | ARG A | | 65.623 | | 116.225 | 1.00 36.07 |
| MOTA | 2417 | С | ARG A | 304 | 61.585 | | 120.803 | 1.00 25.46 |
| MOTA | 2418 | 0 | ARG A | 304 | 61.519 | | 121.876 | 1.00 24.23 |
| ATOM | 2419 | N | ALA A | 305 | 60.741 | 9.854 | 119.802 | 1.00 22.22 |
| ATOM | 2420 | CA | ALA A | | 59.700 | 10.868 | 119.910 | 1.00 26.70 |
| ATOM | 2421 | | ALA A | | 58.914 | 10.960 | 118.607 | 1.00 28.14 |
| MOTA | 2422 | | ALA A | | 58.749 | | 121.072 | 1.00 25.54 |
| | | | | | 58 513 | | 121.883 | 1.00 24.17 |
| ATOM | 2423 | | ALA A | | 58 189 | | 121.160 | 1.00 25.66 |
| MOTA | 2424 | | TRP A | | | | | |
| MOTA | 2425 | | TRP A | | 57.270 | | 122.253 | 1.00 28.01 |
| ATOM | 2426 | | TRP A | | 56.454 | | 122.012 | 1.00 18.66 |
| ATOM | 2427 | | TRP A | | 55.382 | | 120.973 | 1.00 21.80 |
| ATOM | 2428 | CD2 | TRP A | 306 | 54.709 | 7.019 | 120.240 | 1.00 24.88 |
| ATOM | 2429 | | TRP A | | 53.725 | 7.646 | 119.442 | 1.00 23.98 |
| ATOM | 2430 | | TRP A | | 54.839 | | 120.181 | 1.00 23.26 |
| | 2431 | | TRP A | | 54.795 | | 120.599 | 1.00 20.24 |
| MOTA | | | TRP A | | 53.7.99 | | 119.681 | 1.00 24.18 |
| ATOM | 2432 | | | | | | 118.590 | 1.00 24.10 |
| MOTA | 2433 | | TRP A | | 52.875 | | | |
| MOTA | 2434 | | TRP A | | 53.993 | | 119.335 | 1.00 23.89 |
| ATOM | 2435 | | TRP A | | 53.024 | 5.562 | 118.550 | 1.00 24.12 |
| MOTA | 2436 | , C | TKP A | 306 | 57.969 | 9.113 | 123.605 | 1.00 27.93 |
| MOTA | 2437 | · О | TRP A | 306 | 57.330 | 9.319 | 124.637 | 1.00 28.58 |
| ATOM | 2438 | | THR A | | 59.273 | 8.851 | 123.615 | 1.00 26.76 |
| | 2439 | CA | THR A | 307 | 60.000 | 8 850 | 124.881 | 1.00 22.81 |
| ATOM | 2440 | CP | THR A | 307 | 61.457 | 8 319 | 124.730 | 1.00 25.54 |
| ATOM | | CB | TUV V | 307 | 61.435 | 6.313 | 124.504 | 1.00 22.73 |
| ATOM | 2441 | OGI | THR A | 207 | | 0.502 | 125 000 | 1.00 24.03 |
| ATOM | 2442 | CG2 | THR A | 307 | 62.269 | 8.599 | 125.988 | 1.00 24.03 |

| ATOM | 1 2443 C THR A 307 | 60.027 10.288 125.396 1 00 26 54 |
|---------------|--|--|
| ATOM | 1 2444 O THRA 307 | 60.027 10.288 125.396 1.00 26.54 59.925 10.526 126.604 1.00 25.34 |
| ATOM | 1. 500 | 60.152 11.247 124.478 1.00 21.65 |
| ATOM ATOM | | 60.172 12.657 124.862 1.00 21 41 |
| ATOM | | 60.442 13.558 123.642 1.00 19.20 |
| ATOM | | 61./9/ 13.386 122.938 1.00 21.31 |
| ATOM | | 61.900 14.362 121.774 1.00 21.75 |
| ATOM | 1. 500 | 62.937 13.622 123.915 1.00 19.26 58.811 12.981 125.479 1.00 25.18 |
| ATOM | | |
| ATOM | 2453 N ILE A 309 | |
| ATOM | 2454 CA. ILE A 309 | 57.743 12.567 124.806 1.00 21.74 56.394 12.799 125.298 1.00 19.23 |
| MOTA | | 55.337 12.149 124.366 1.00 19.63 |
| MOTA | | 53.945 12.321 124.948 1 00 19 54 |
| MOTA MOTA | | 55.403 12.788 122.979 1.00 20.80 |
| ATOM | 1. 505 | 55.118 14.274 122.988 1.00 20.08 |
| ATOM | 2460 O ILE A 309 | 56.228 12.222 126.701 1.00 23.97 |
| ATOM | 2461 N TRP A 310 | 55.731 12.894 127.602 1.00 21.38 56.652 10.977 126.888 1.00 26.45 |
| ATOM | 2462 CA TRP A 310 | |
| ATOM | 2463 CB TRP A 310 | 56.525 10.342 128.192 1.00 28.35 56.940 8.872 128.132 1.00 23.95 |
| ATOM | 2464 CG TRP A 310 | 56.874 8.203 129.479 1.00 29.60 |
| MOTA | 2465 CD2 TRP A 310 | 55.697 7.967 130.263 1.00 31 40 |
| ATOM- ATOM | 2466 CE2 TRP A 310 2467 CE3 TRP A 310 | 56.115 7.390 131.480 1.00 32.47 |
| MOTA | 2467 CE3 TRP A 310 2468 CD1 TRP A 310 | 54.329 8.189 130.055 1.00 32.30 |
| ATOM | 2469 NEI TRP A 310 | 57.926 7.770 130.232 1.00 33.42 57.480 7.282 131.436 1.00 30.09 |
| ATOM | 2470 CZ2 TRP A 310 | == ==================================== |
| MOTA | 2471 CZ3 TRP A 310 | 23,33 |
| ATOM | 2472 CH2 TRP A 310 | 53.432 7.831 131.062 1.00 29.72 53.881 7.259 132.265 1.00 24.53 |
| ATOM | 2473 C TRP A 310 | 57.308 11.048 129.293 1.00 33.49 |
| MOTA | 2474 O TRP A 310 | 56.820 11.137 130.426 1.00 27.59 |
| ATOM ATOM | 2475 N CYS A 311 2476 CA CYS A 311 | 58.512 11.535 128.984 1.00 29.34 |
| ATOM | 2476 CA CYS A 311 2477 CB CYS A 311 | 59.305 12.247 129.994 1.00 30.06 |
| ATOM | 2478 SG CYS A 311 | 60.722 12.538 129.479 1.00 30.08 61.804 11.084 129.327 1.00 33.17 |
| MOTA | 2479 C CYS A 311 | |
| ATOM | 2480 O CYS A 311 | 58.612 13.560 130.397 1.00 29.25 58.612 13.940 131.570 1.00 28.80 |
| MOTA | 2481 N GLU A 312 | 58.021 14.247 129.425 1.00 23.13 |
| ATOM | 2482 CA GLU A 312 | 57.308 15.496 129.696 1.00 30.31 |
| ATOM ATOM | 2483 CB GLU A 312 2484 CG GLU A 312 | 56.648 16.032 128.427 1.00 28.97 |
| ATOM | 2484 CG GLU A 312 2485 CD GLU A 312 | 57.080 17.418 127.988 1.00 41.67 |
| ATOM | 2486 OE1 GLU A 312 | 56.905 18.465 129.059 1.00 44.21 55.813 18.534 129.658 1.00.54.15 |
| ATOM | 2487 OE2 GLU A 312 | 55 050 |
| MOTA | 2488 C GLU A 312 | |
| MOTA | 2489 O GLU A 312 | 56.204 15.225 130.712 1.00 28.03 56.120 15.869 131.751 1.00 30.64 |
| ATOM | 2490 N LEU A 313 | 55.343 14.270 130.388 1.00 31.06 |
| MOTA | 2491 CA LEU A 313 | 54.231 13.918 131.266 1.00 36.21 |
| ATOM ATOM | 2492 CB LEU A 313 2493 CG LEU A 313 | 53.337 12.873 130.604 1.00 28.83 |
| ATOM | 2493 CG LEU A 313 2494 CD1 LEU A 313 | 52.493 13.342 129.429 1.00 34.62 |
| ATOM | 2495 CD2 LEU A 313 | 51.818 12.146 128.788 1.00 33.05 51.471 14.357 129.914 1.00 27 27 |
| ATOM | 2496 C LEU A 313 | |
| MOTA | 2497 O LEU A 313 | |
| MOTA | 2498 N SER A 314 | 54.131 13.730 133.644 1.00 37.26 55.688 12.508 132.577 1.00 33.72 |
| MOTA | 2499 CA SER A 314 | 56.233 11.880 133.776 1.00 33.58 |
| ATOM | 2500 CB SER A 314 | 57.183 10.743 133.388 1.00 35.88 |
| MOTA | 2501 OG SER A 314 | 56.517 9.761 132.628 1.00 45.88 |
| atom Atom | 2502 C SER A 314 2503 O SER A 314 | 57.002 12.846 134.659 1.00 31.54 |
| ATOM ATOM | 2504 N GLY A 315 | 57.339 12.513 135.788 1.00 27.69 57.312 14.021 134.130 1.00 35.50 |
| TCM | 2505 CA GLY A 315 | |
| MOTA | 2506 C GLY A 315 | 50 510 |
| ATCM | 2507 O GLY A 315 | 59.518 14.634 135.099 1.00 38.47 60.138 15.049 136.078 1.00 41.57 |
| MOTA | 2508 N ARG A 316 | 60.089 13.862 134.181 1.00 39.32 |
| | | 1.00 33.32 |



| | | | | ' - ' | | |
|--------------|--------------|----------|------------------------|------------------|----------------------------------|--------------------------|
| ATOM | 2509 | CA | ARG A 316 | 61.490 | 13.501 134.332 | 1.00 39.06 |
| MOTA | 2510 | CB | ARG A 316 | 61.641 | 11.982 134.413 | 1.00 39.16 |
| MOTA | 2511 | CG | ARG A 316 | 61.233 | 11.226 133.184 | 1.00 39.11 |
| MOTA | 2512 | CD | ARG A 316 | 61.426 | 9.744 133.429 | 1.00 41.21 |
| MOTA | 2513 | NE | ARG A 316 | 60.461 | 9.229 134.389 | 1.00 40.97 |
| ATOM- | 2514 | CZ | ARG A 316 | 60.524 | 8.021 134.926 | 1.00 36.40 |
| ATOM | 2515 | NH1 | ARG A 316 | 61.511 | 7.209 134.598 | 1.00 38.93 |
| MOTA | 2516 | NH2 | ARG A 316 | 59.583 | 7.621 135.768 | 1.00 30.53 |
| ATOM | 2517 | С | ARG A 316 | 62.369 | 14.083 133.230 | 1.00 40.17 |
| MOTA | 2518 | 0 | -ARG A 316 | 61.910 | 14.325 132.111 | 1.00 34.27 |
| MOTA | 2519 | N | GLU A 317 | 63.633 | 14.325 133.564 | 1.00 41.26 |
| ATOM | 2520 | CA | GLU A 317 | 64.580 | 14.905 132.619 | 1.00 44.42 |
| ATOM | 2521 | CB | GLU A 317 | 65.901 | 15.249 133.317 | 1.00 46.84 |
| ATOM | 2522 | CG | GLU A 317 | 65.756 | 15.996 134.629 | 1.00 57.66 |
| ATOM | 2523 | CD | GLU A 317 | 65.212 | 15.113 135.743 14.101 136.073 | 1.00 65.46 |
| MOTA | 2524 | OE1 | GLU A 317 | 65.871 | | 1.00 68.38 |
| MOTA | 2525 2526 | OE2 C | GLU A 317 | 64.129 64.873 | 15.425 136.287 13.962 131.462 | 1.00 67.24 |
| ATOM ATOM | 2527 | 0 | GLU A 317 GLU A 317 | 64.977 | 12.748 131.636 | 1.00 38.45 |
| ATOM | 2528 | N | VAL A 318 | 65.010 | 14.525 130.275 | 1.00 37.64 |
| ATOM | 2529 | CA | VAL A 318 | 65.315 | 13.720 129.108 | 1.00 39.13 |
| ATOM | 2530 | CB | VAL A 318 | 64.858 | 14.417 127.810 | 1.00 42.75 |
| ATOM | 2531 | CG1 | | 65.192 | 13.544 126.610 | 1.00 41.84 |
| ATOM | 2532 | CG2 | VAL A 318 | 63.364 | 14.701 127.867 | 1.00 42.38 |
| ATOM | 2533 | C | VAL A 318 | 66.822 | 13.495 129.037 | 1.00 38.45 |
| ATOM | 2534 | 0 | VAL A 318 | 67.598 | 14.442 128.910 | 1.00 36.04 |
| ATOM | 2535 | N | PRO A 319 | 67.261 | 12.236 129.156 | 1.00 39.54 |
| ATOM | 2536 | CD | PRO A 319 | • 66.512 | 10.994 129.397 | 1.00 40.47 |
| ATOM | 2537 | CA | PRO A 319 | 68.695 | 11.949 129.088 | 1.00 43.85 |
| MOTA | 2538 | CB | PRO A 319 | . 68.745 | 10.439 129.319 | 1.00 44.12 |
| MOTA | 2539 | CG | PRO A 319 | 67.419 | 9.986 128.745 | 1.00 46.48 |
| MOTA | 2540 | c | PRO A 319 | 69.228 | 12.353 127.718 | 1.00 43.55 |
| MOTA | 2541 | 0 | PRO A 319 | 68.563 | 12.141 126.708 | 1.00 43.45 |
| ATOM | 2542 | N | GLU A 320 | 70.420 71.026 | 12.936 127.689 | 1.00 42.52 1.00 45.19 |
| ATOM | 2543 | CA CB | GLU A 320 GLU A 320 | 72.384 | 13.380 126.440 14.032 126.706 | 1.00 43.19 |
| ATOM ATOM | 2544 2545 | CG | GLU A 320 | 73.121 | 14.412 125.434 | 1.00 52.62 |
| ATOM | 2546 | CD | GLU A 320 | 74.507 | 14.967 125.697 | 1.00 52.36 |
| ATOM | 2547 | OE1 | | 75.219 | 15.271 124.720 | 1.00 56.25 |
| | . 2548 | OE2 | GLU A 320 | 74.883 | 15.101 126.875 | 1.00 52.25 |
| ATOM | 2549 | C | GLU A 320 | 71.223 | 12.266 125.421 | 1.00 43.52 |
| ATOM | 2550 | 0 | GLU A 320 | 70.876 | 12.412 124.253 | 1.00 41.89 |
| ATOM | 2551 | N | LYS A 321 | 71.781 | 11.150 125.867 | 1.00 43.35 |
| MOTA | 2552 | CA | LYS A 321 | 72.059 | 10.041 124.969 | 1.00 43.53 |
| ATOM | 2553 | CB | LYS A 321 | 73.561 | 9.808 124.879 | 1.00 42.78 |
| ATOM | 2554 | CG | LYS A 321 | 74.238 | 9.34C 126.180 | 1.00 49.38 |
| MOTA | 2555 | CD | LYS A 321 | 74.272 | 10.396 127.307 | 1.00 57.82 |
| ATOM | 2556 | CE. | LYS A 321 | 72.978 | 10.497 128.129 | 1.00 53.81 |
| ATOM | 2557 | | LYS A 321 | 72.660 71.407 | 9.245 128.883 8.731 125.345 | 1.00 54.17 1.00 41.52 |
| ATOM | 2558 | | LYS A 321 | 70.954 | 8.540 126.469 | 1.00 41.52 |
| ATOM | 2559 | | LYS A 321 LEU A 322 | 71.378 | 7.820 124.382 | 1.00 38.64 |
| MOTA | 2560 2561 | | LEU A 322 | 70.815 | 6.508 124.613 | 1.00 40.46 |
| ATOM | 2562 | | LEU A 322 | 70.442 | 5.845 123.289 | 1.00 42.22 |
| MOTA MOTA | 2563 | | LEU A 322 | 69.595 | 6.632 122.287 | 1.00 42.92 |
| ATOM | 2564 | | LEU A 322 | 69.204 | 5.737 121.125 | 1.00 41.13 |
| MOTA | 256.5 | | LEU A 322 | 68.361 | 7.148 122.967 | 1.00 44.41 |
| ATOM | 2566 | C | LEU A 322 | 71.918 | 5.702 125.268 | 1.00 41.36 |
| ATOM | 2567 | ō | LEU A 322 | 73.079 | 5.825 124.884 | 1.00 44.16 |
| ATOM | 2568 | N | ASN A 323 | 71.579 | 4.894 126.265 | 1.00 39.89 |
| MOTA | 2569 | CA | ASN A 323 | 72.594 | 4.067 126.895 | 1.00 40.96 |
| ATOM | 2570 | CB | ASN A 323 | 72.136 | 3.556 128.259 | 1.00 43.00 |
| ATOM | 2571 | CG | ASN A 323 | 70.787 | 2.886 128.202 | 1.00 45.59 |
| ATOM | 2572 | OD1 | ASN A 323 | 70.482 | 2.151 127.264 | 1.00 45.71 |
| ATOM | 2573 | ND2 | ASN A 323 | 69.975 | 3.114 129.224 | 1.00 48.08 |
| ATOM | 2574 | | ASN A 323 | 72.828 | 2.894 125.954 | 1.00 44.88 |

| | _ | _ |
|------|-----------------------|--|
| AT | TOM 2575 O ASN A 323 | 72 424 |
| AT | COM 2576 N ASN A 324 | 72.124 2.739 124.955 1.00 46.4 |
| ΓA | OM 2577 CA ASN A 324 | 73.809 2.062 126.268 1 00 45 0 |
| . AT | OM 2578 CB ASN A 324 | 79.122 0.938 125.404 1 00 40 0 |
| AT | OM 2579 CG ASN A 324 | 75.386 0.244 125 904 1 00 53 6 |
| | OM 2580 OD1 ASN A 324 | /5.960 -0.711 124.888 1 00 60 0 |
| | OM 2581 ND2 ASN A 324 | /5.344 -1.723 124.550 1 00 66 0 |
| | OM 2582 C ASN A 324 | 77.143 -0.386 124.378 1 00 50 0 |
| AT | ASM A 324 | 72.979 -0.070 125.267 1 00 47 13 |
| AT | 10N W.324 | 72.784 -0.644 124.197 1 00 43 63 |
| ATO | DID A 343 | 72.220 -0.276 126.339 1 00 46 36 |
| ATC | DIS A 323 | . /1.106 -1.221 126.318 1 00 46 76 |
| ATO | - DID A 323 | 70.428 -1.328 127.695 1 00 47 65 |
| ATC | DID N 323 | /1.292 -1.837 128.858 1 00 54 21 |
| ATO | 02 1313 R 323 | 72.160 -0.750 129.526 1 00 56 87 |
| ATC | , 0_ DIS A 323 | /3.329 -0.289 128.671 1.00 57 45 |
| ATC | 215 A 325 | 74.091 0.816 129.307 1 00 58 33 |
| ATO | 213 A 323 | 70.062 -0.791 125 296 1 00 45 15 |
| ATO | 215 A 323 | 69.474 -1.625 124.601 1 00 42 72 |
| ATO | A 320 | 69.832 0.514 125 213 1 00 41 43 |
| ATO | 111A A 326 | 68.861 1.054 124 276 1 00 41 61 |
| ATO | | 50 550 0 1.00 41.61 |
| | FUA A 320 | 69.365 0.940 122 838 1 00 42 00 |
| ATO | man n 326 | 60 505 |
| ATO | - 215 x 327 | 70 550 1 1.00 45.1/ |
| ATO | DID A 34/ | 71 225 |
| ATO | 210 N J2/ | 70 700 |
| ATO | 210 x 32/ | 77 078 |
| ATO | 210 A 32/ | 74 544 - 1-1000 1.00 30.87 |
| ATON | A10 A 32/ | 24 046 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| ATOM | 110 BIS R 321 | 74 055 |
| ATOM | C DIS R 32/ | 71 050 |
| ATOM | 315 A 347 | |
| ATOM | - OLO A 328 | 71 402 1.00 38.83 |
| MOTA | 525 A 528 | 71 276 |
| ATOM | | 71 000 |
| ATOM | -0 CAC A 326 | 72 260 1100 43.05 |
| ATOM | 420 A 326 | 74 006 |
| ATOM | CLO A 328 | 77 077 |
| ATOM | 2613 OE2 GLU A 328 | 74 75- |
| ATOM | 2614 C GLU A 328 | 60 025 2 020 200 21.00 21.04 |
| MOTA | 2615 O GLU A 328 | 60 536 3 646 446 |
| ATOM | 2616 N LEU A 329 | |
| ATOM | 2617 CA LEU A 329 | (2 404 |
| ATOM | 2618 CB LEU A 329 | |
| ATOM | 2619 CG LEU A 329 | Cr 120 - 120 1.00 34.00 |
| ATOM | 2620 CD1 LEU A 329 | |
| ATOM | 2621 CD2 LEU A 329 | 64 30- |
| ATOM | 2622 C LEU A 329 | 57 100 24,00 |
| ATOM | 2623 O LEU A 329 | 26 65 20 33.04 |
| ATOM | 2624 N LEU A 330 | 67 333 |
| MOTA | 2625 CA LEU A 330 | 52 22 1.00 33.78 |
| MOTA | 2626 CB LEU A 330 | |
| ATOM | 2627 CG LEU A 330 | 20.234 1.00 30.74 |
| ATOM | 2628 CD1 LEU A 330 | 56 055 |
| ATOM | 2629 CD2 LEU A 330 | Cr 000 |
| ATOM | 2630 C LEU A 330 | 62 20 1.00 29.69 |
| ATOM | 2631 O LEU A 330 | 57 149 1.00 36.49 |
| ATOM | 2632 N LYS A 331 | 50 005 |
| ATCM | 2633 CA LYS A 331 | 60 306 |
| ATOM | 2634 CB LYS A 331 | 71 250 1100 1100 41.32 |
| ATOM | 2635 CG LYS A 331 | 71 004 |
| ATOM | 2636 CD LYS A 331 | 77 750 1.00 44.08 |
| ATOM | 2637 CE LYS A 331 | 74.350 -0.964 117.498 1.00 51.42 |
| ATOM | 2638 NZ LYS A 331 | 73.030 -1.889 116.765 1.00 53.71 |
| ATCH | 2639 C LYS A 331 | 73.928 -3.327 116.855 1.00 56.15 |
| ATOM | 2640 O LYS A 331 | 69.258 -3.612 116.173 1.00 42.35 |
| | PID V 23T | 69.310 -4.086 115.042 1.00 42.68 |
| | | - |

```
-4.270 117.200
                                                             1.00 41.56
                                   68.734
       2641
              N
                  SER A 332
MOTA
                                           -5.629 117.039
                                                             1.00 46.88
                                   68.226
                  SER A 332
       2642
              CA
ATOM
                  SER A 332
                                   68.045
                                           -6.298 118.400
                                                             1.00 42.19
       2643
              CR
MOTA
                                   66.959
                                           -5.714 119.096
                  SER A 332
MOTA
       2644
              OG
                                           -5.687 116.297
                                                             1.00 48.58
                                   66.896
       2645
              C
MOTA
                                   66.393
                                           -6.774 116.017
                                                             1.00 45.78
       2646
                  SER A 332
              O
MOTA
                                           -4.531 115.979
                                   66.325
                                                             1.00 48.27
                  ILE A 333
       2647
              N
ATOM
                                           -4.503 115.292
                                                             1.00 51.82
                  ILE A 333
                                   65.041
       2648
              CA
MOTA
                                   64.378
                                                   115.402
                                                             1.00 52.16
                  ILE A 333
                                           -3.119
       2649
              CB
MOTA
                                   63.038
                                           -3.122 114.683
                                                             1.00 52.64
       2650
              CG2
                  ILE A 333
ATOM
                                           -2.765 116.871
                                                             1.00 52.70
              CG1
                  ILE A 333
                                   64.163
       2651
ATOM
                                   63.550
                                           -1.402 117.077
                                                             1.00 56.70
              CD1
                  ILE A 333
       2652
ATOM
                                   65.112
                                           -4.887 113.820
                                                             1.00 53.43
       2653
                  ILE A 333
              C
MOTA
                                                             1.00 56.45
                                           -4.675 113.145
                                   66.118
       2654
              0
                  ILE A 333
ATOM
                                   64.016
                                           -5.461 113.344
                                                             1.00 55.53
                  ASP A 334
       2655
              N
MOTA
                                           -5.892 111.962
                                                             1.00 59.58
                                   63.865
       2656
                  ASP A 334
              CA
ATOM
                                                             1.00 62.69
                                           -7.040 111.918
                                   62.845
       2657
              CB
                  ASP A 334
MOTA
                  ASP A 334
                                   61.546
                                            -6.712 112.664
                                                             1.00 66.23
       2658
              CG
ATOM
                                           -5.814 112.227
-7.354 113.704
                                   60.795
                                                             1.00 63.25
       2659
              OD1
                  ASP A 334
ATOM
                                                             1.00 63.45
                                   61.277
                  ASP A 334
       2660
              OD2
MOTA
                                            -4.705 111.125
                  ASP A 334
                                   63.385
                                                             1.00 60.81
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              С
ATOM
                                   62.239
                                            -4.673 110.681
                                                             1.00 59.47
       2662
              0
                  ASP A 334
MOTA
                                           -3.736 110.889
                                                             1.00 60.00
                                   64.266
                  PHE A 335
       2663
              N
ATOM
                                                             1.00 59.37
                                                   110.147
                  PHE A 335
                                   63.864
                                            -2.545
              CA
ATOM
       2664
                                   64.247
                                            -1.298
                                                   110.952
                                                             1.00 53.38
                  PHE A 335
       2665
              CB
ATOM
                                                   110.275
                                                             1.00 49.13
                                   63.895
                                            ~0.013
       2666
              CG
                  PHE A 335
MOTA
                                                   109.770
                                                             1.00 44.32
                                   62.618
                                             0.189
       2667
              CD1
                  PHE A 335
MOTA
                                                             1.00 49.91
                                   64.845
                                             0.993 110.127
       2668
                  PHE A 335
              CD2
ATOM
                                   62.288
                                             1.373
                                                   109.122
                                                             1.00 42.74
                  PHE A 335
       2669
              CE1
MOTA
                                   64.526
                                             2.180 109.483
                                                             1.00 46.40
       2670
              CE2
                  PHE A 335
MOTA
                                             2.370 108.978
                                                             1.00 42.77
                  PHE A 335
                                   63.244
       2671
              CZ
ATOM
                                                             1.00 60.85
                                   64.334
                                            -2.399
                                                   108.696
                  PHE A 335
ATOM
       2672
              C
                                            -2.914 107.785
                                                              1.00 66.28
                                   63.689
       2673
              O
                  PHE A 335
MOTA
                                           -1:671 108.493
                                                              1.00
                                                                   57.40
                                   65.430
                  GLU A 336
       2674
MOTA
                                            -1.411 107.174
                                                              1.00 58.96
                  GLU A 336
       2675
                                   66.015
              CA
ATOM
                                            -2.579 106.211
                                                              1.00 62.66
                                   65.782
                  GLU A 336
ATOM
       2676
              CB
                                   66.417
                                                   104.846
                                                              1.00 68.51
                                            -2.377
       2677
                  GLU A 336
              CG
MOTA
                                            -3.590 103.943
                                                              1.00 73.21
                  GLU A 336
                                   66.277
              CD
       2678
ATOM
                                                              1.00 73.30
                                   66.753
                                            -4.678 104.333
                  GLU A 336
       2679
              OF1
MOTA
                                            -3.457 102.843
                                                              1.00 75.74
                                   65.697
                  GLU A 336
       2680
              OE2
MOTA
                                                              1.00 55.70
                                            -0.124 106.576
                                   65.460
                  GLU A 336
       2681
              C
MOTA
                                                              1.00 55.28
                                            -0.023 106.253
                  GLU A 336
                                   64.281
       2682
MOTA
              o
                                                              1.00 54.75
                                   66.338
                                             0.857 106.432
                  GLU A 337
       2683
              N
MOTA
                                             2.167 105.905
                                                              1.00 55.99
                                   65.986
              CA
                  GLU A 337
       2684
MOTA
                                             3.065 105.983
                                                              1.00 51.75
                                   67.221
                  GLU A 337
              CB
ATOM
       2685
                                             4.536 106.092
                                                              1 00 52.28
                                   66.926
                  GLU A 337
             CG
       2686
ATOM
                                             4.891 107.366
                                                               .00 43.72
                                   66.184
       2687
              CD
                  GLU A 337
MOTA
                                             4.640
                                   66.705
                                                   108.474
                                                               00 42.21
                  GLU A 337
       2688
MOTA
                                             5.425 107.256
                                                              1.00 47.31
              OE2
                  GLU A 337
                                   65.072
       2689
ATOM
                                                              1.00 57.56
                                             2.064 104.460
                                   65.485
                  GLU A 337
ATOM
       2690
              С
                                   66.087
                                             1.377
                                                   103.639
                                                              1.00 58.29
                  GLU A 337
       2691
MOTA
                                             2.745 104.151
                                                              1.00 60.26
                  PHE A 338
                                   64.385
             N
       2692
ATOM
                                                              1.00 61.69
                                             2.710 102.805
                                   63.814
                  PHE A 338
ATOM
       2693
             CA
                                   62.561
                                             3.582
                                                   102.723
                                                              1.00 60.86
                  PHE A 338
       2694
ATOM
                                             3.493 101.401
                                                              1.00 61.92
                                   61.845
             CG
                  PHE A 338
       2695
MOTA
                                             2.391 101.094
                                                              1.00 62.99
                  PHE A 338
                                   61.054
             CD1
       2696
ATOM
                                   61.970
                                             4.508 100.458
                                                              1.00 62.74
             CD2
                  PHE A 338
       2697
ATOM
                                             2.302
                                                    99.868
                                                              1.00 65.11
                  PHE A 338
                                   60.392
             CE1
       2698
ATOM
                                                     99.228
                                                              1.00 64.62
                                             4.428
                  PHE A 338
                                   61.315
       2699
             CE2
MOTA
                                   60.523
                                             3.322
                                                     98.934
                                                              1.00 63.87
                  PHE A 338
       2700
             CZ
ATOM
                                             3.208 101.773
                                                              1.00 64.33
                                   64.818
       2701
                  PHE
                      A 338
             C
ATOM
                                             2.781 100.616
                                                              1.00 62.45
                                   64.803
                  PHE A 338
       2702
             0
ATOM
                                   65.677
                                             4.130
                                                   102.194
                                                              1.00 64.11
                  ASP A 339
       2703
             N
ATOM
                                             4.684 101.310
                                                              1.00 67.42
                  ASP
             CA
                      A 339
                                   66.689
       2704
MOTA
                                             6.206 101.248
                                                              1.00 67.20
                  ASP
                      A 339
                                   66.565
       2705
             ÇB
ATCM
                  ASP A 339
                                             6.838 100.402
                                                              1.00 68.03
                                   67.647
       2706
ATCM
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| ATOM | 4 2707 OD1 ASP A 339 | 67.796 6.432 99.229 1 00 72 20 |
|-------|----------------------|---|
| ATOM | | 1.00 72.20 |
| ATOM | | 7.00 04.13 |
| ATOM | - 1121 11 303 | 68.088 4.295 101.763 1.00 68.73 |
| ATOM | | 08.511 4.628 102.869 1.00 68.17 |
| | | 00./90 3.588 100.888 1 nn-71 an |
| ATOM | | 70.151 3.111 101.149 1 00 73 50 |
| ATOM | | 70.778 2.601 99.848 1.00 75.47 |
| MOTA | | 70 |
| ATOM | 1 2715 OD1 ASP A 340 | 50 75 75 75 75 75 75 75 75 75 75 75 75 75 |
| ATOM | | 50 100 76.90 |
| ATOM | 2717 C ASP A 340 | 71 000 |
| ATOM | 0.0 | 71 500 12.11 |
| MOTA | | 71.018 3.946 102.845 1.00 73 09 |
| ATOM | 000 11 331 | 71.242 5.275 101.074 1.00 73 15 |
| | | 72.112 6.341 101.557 1.00 74 56 |
| ATOM | | 72.917 6.924 100.390 1 00 77 06 |
| ATOM | | 73.878 8.034 100.792 1 00 92 57 |
| MOTA | | 74.924 7.571 101.794 1.00 85.34 |
| ATOM | | |
| ATOM | 2725 OE2 GLU A 341 | |
| ATOM | 2726 C GLU A 341 | |
| ATOM | . 2727 O GLU A 341 | 72.47 |
| ATOM | | 71 00- |
| ATOM | | |
| ATOM | 2730 CB VAL A 342 | 70.503 8.393 104.323 1.00 64.84 |
| ATOM | 2731 CG1 VAL A 342 | 69.160 7.853 104.850 1.00 66.27 |
| ATOM | 2732 CG2 VAL A 342 | 68.256 7.494 103.701 1.00 67 95 |
| ATOM | 2733 C VAL A 342 | 93.400 6.637 105.722 1.00 65 37 |
| | | 71.305 8.871 105.520 1.00 61 75 |
| ATOM | | /1.3/5 10.066 105.795 1.00 64 14 |
| ATOM | 2735 N ASP A 343 | 71.912 7.925 106.225 1.00 56.79 |
| ATOM- | 11 343 | 72.692 8.229 107.417 1 00 54 52 |
| MOTA | 2737 CB ASP A 343 | 73.707 9.340 107.158 1 00 56 31 |
| MOTA | 2738 CG ASP A 343 | 74.531 9.660 108.388 1.00 58.81 |
| ATOM | 2739 OD1 ASP A 343 | 75.298 10.644 108.357 1.00 65.36 |
| MOTA | 2740 OD2 ASP A 343 | |
| ATOM | 2741 C ASP A 343 | 2.00 34.29 |
| MOTA | 2742 O ASP A 343 | |
| ATOM | 2743 N ARG A 344 | |
| ATOM | 2744 CA ARG A 344 | 70 455 |
| MOTA | 2745 CB ARG A 344 | 1.00 41.10 |
| ATOM | 2746 CG ARG A 344 | 1.00 39.81 |
| ATOM | 2747 CD ARG A 344 | 1.00 33.00 |
| ATOM | 2748 NE ARG A 344 | 68.036 9.211 109.121 1.00 28.37 |
| ATOM | 2749 CZ ARG A 344 | 67.157 9.645 108.036 1.00 30.90 |
| ATOM | | 67.013 10.909 107.649 1.00 31.05 |
| | | 67.693 11.874 108.258 1.00 30 40 |
| ATOM | | 66.201 11.212 106.646 1.00 31 76 |
| MOTA | | 71.147 7.561 111.742 1.00 38.46 |
| ATOM | 2753 O ARG A 344 | 70.516 7.370 112.773 1 00 34 00 |
| ATOM | 2754 N SER A 345 | 7.418 111.662 1.00 33 97 |
| MOTA | 2755 CA SER A 345 | 73.261 6.981 112.795 1.00 33.68 |
| MOTA | 2756 CB SER A 345 | 74.742 6.972 112.404 1.00 39.11 |
| MOTA | 2757 OG SER A 345 | 75.163 8.260 111.990 1.00 42.80 |
| ATOM | 2758 C SER A 345 | |
| ATOM | 2759 O SER A 345 | 1.00 11.83 |
| ATOM | 2760 N TYR A 346 | |
| MOTA | 2761 CA TYR A 346 | |
| MOTA | 2762 CB TYR A 346 | |
| MOTA | 2763 CG TYR A 346 | |
| MOTA | 2764 CD1 TYR A 346 | 71.168 11.615 113.659 1.00 39.69 |
| ATOM | | 69.909 11.814 114.227 1.00 36.57 |
| | | 68./6/ 11.940 113.424 1.00 40.23 |
| MOTA | | /1.200 11.544 112.270 1.00 39.04 |
| ATOM | | 70.131 11.667 111.463 1.00 38.65 |
| TOM | 2768 CZ TYR A 346 | 68.890 11.864 112.041 1.00 37.64 |
| TOM | 2769 OH TYR A 346 | 67.776 11.982 111.234 1.00 32 48 |
| MOT | 2770 C TYR A 346 | 71.432 9.560 115.874 1.00 37 72 |
| TCM | 2771 O TYR A 346. | 71.396 9.829 117.074 1.00 35.48 |
| TCM | 2772 N MET A 347 | 70.472 8.869 115.265 1.00 35.36 |
| | - | 2.00 33.36 |

Figure 18-43

| ATOM | 2773 | CA | MET A 347 | | 69.295 | 8.418 | 116.004 | 1.00 36.97 |
|--------|------|-----|-------------|---|--------|--------|--------------------|------------|
| MOTA | 2774 | CB | MET A 347 | | 68.226 | 7.868 | 115.052 | 1.00 33.45 |
| ATOM | 2775 | CG | MET A 347 | | 67.853 | | 113.921 | 1.00 28.09 |
| ATOM | 2776 | SD | MET A 347 | | 66.471 | | 112.943 | 1.00 32.14 |
| MOTA | 2777 | CE | MET A 347 | | 67.058 | | 112.457 | 1.00 39.25 |
| | 2778 | C | MET A 347 | | 69.632 | | 117.055 | 1.00 34.67 |
| ATOM- | | | | | 68.890 | | 118.016 | 1.00 33.46 |
| MOTA | 2779 | 0 | MET A 347 | | | | 116.880 | |
| MOTA | 2780 | N | LEU A 348 | | 70.747 | | | 1.00 36.42 |
| MOTA | 2781 | CA | LEU A 348 | | 71.137 | | 117.846 | 1.00 34.57 |
| MOTA | 2782 | CB | -LEU A 348 | | 71.841 | | 117.152 | 1.00 34.16 |
| MOTA | 2783 | CG | LEU A 348 | | 71.066 | | 116.121 | 1.00 35.61 |
| MOTA | 2784 | CD1 | L LEU A 348 | | 72.010 | | 115.469 | 1.00 36.58 |
| MOTA | 2785 | CD2 | | • | 69.906 | | 116.788 | 1.00 42.34 |
| MOTA | 2786 | С | LEU A 348 | | 72.075 | | 118.885 | 1.00 37.10 |
| ATOM | 2787 | 0 | LEU A 348 | | 72.583 | 5.513 | 119.745 | 1.00 37.75 |
| MOTA | 2788 | N | GLU A 349 | | 72.295 | 7.541 | 118.801 | 1.00 38.31 |
| MOTA | 2789 | CA | GLU A 349 | | 73.192 | 8.231 | 119.726 | 1.00 42.86 |
| ATOM | 2790 | CB | GLU A 349 | | 74.150 | 9.136 | 118.948 | 1.00 47.04 |
| ATOM | 2791 | CG | GLU A 349 | | 74.942 | 8.426 | 117.867 | 1.00 53.27 |
| ATOM | 2792 | CD | GLU A 349 | | 75.828 | 7.325 | 118.410 | 1.00 58.36 |
| ATOM | 2793 | OE1 | | | 76.681 | 7.619 | 119.279 | 1.00 59.59 |
| ATOM | 2794 | OE2 | | | 75.669 | | 117.963 | 1.00 59.17 |
| ATOM | 2795 | c | GLU A 349 | | 72.458 | | 120.752 | 1.00 41.72 |
| ATOM | 2796 | ŏ | GLU A 349 | | 72.564 | | 121.959 | 1.00 42.27 |
| ATOM | 2797 | N | THR A 350 | | 71.716 | | 120.261 | 1.00 37.05 |
| ATOM | 2798 | CA | THR A 350 | | 70.992 | | 121.135 | 1.00 40.78 |
| | 2799 | CB | THR A 350 | | 71.468 | | 120.900 | 1.00 41.69 |
| MOTA | 2800 | OG1 | | | 71.359 | | 119.508 | 1.00 43.25 |
| MOTA | 2801 | CG2 | | | 72.918 | | 121.325 | 1.00 44.11 |
| ATOM | 2802 | C | THR A 350 | | 69.474 | | 120.968 | 1.00 41.47 |
| MOTA | 2803 | ō | THR A 350 | • | 68.968 | | 119.884 | 1.00 39.72 |
| MOTA | 2803 | N | LEU A 351 | | 68.760 | | 122.054 | 1.00 38.68 |
| MOTA | | CA | LEU A 351 | | 67.299 | | 122.056 | 1.00 35.91 |
| MOTA | 2805 | | LEU A 351 | | 66.763 | | 123.487 | 1.00 35.94 |
| ATOM | 2806 | CB | | | 66.752 | | 124.251 | 1.00 37.67 |
| ATOM | 2807 | CG | LEU A 351 | | 66.290 | | 125.677 | 1.00 37.07 |
| MOTA | 2808 | | LEU A 351 | | | | 123.544 | 1.00 39.29 |
| MOTA | 2809 | | LEU A 351 | | 65.813 | | 121.294 | 1.00 37.76 |
| MOTA | 2810 | С | LEU A 351 | | 66.679 | | 120.512 | 1.00 34.86 |
| MOTA | 2811 | 0 | LEU A 351 | | 65.747 | | 121.525 | 1.00 34.79 |
| ATOM | 2812 | N | LYS A 352 | | 67.192 | | 120.870 | 1.00 34.73 |
| ATOM | 2813 | CA | LYS A 352 | | 66.651 | | | 1.00 36.48 |
| ATOM | 2814 | CB | LYS A 352 | | 66.676 | | 121.835 | 1.00 38.48 |
| MOTA | 2815 | CG | LYS A 352 | | 66.062 | | 123.179 124.196 | 1.00 43.22 |
| MOTA | 2816 | CD | LYS A 352 | | 66.202 | | | 1.00 49.81 |
| MOTA | 2817 | CE | LYS A 352 | | 65.349 | | 123.845 | |
| MOTA | 2818 | NZ | LYS A 352 | | 65.342 | | 124.972 | 1.00 52.70 |
| MOTA | 2819 | C | LYS A 352 | | 67.425 | | 119.610 | 1.00 38.77 |
| MOTA | 2820 | 0 | LYS A 352 | | 68.654 | | 119.601 | 1.00 36.21 |
| ATOM | 2821 | N | ASP A 353 | | 66.697 | 15.293 | 118.530 | 1.00 37.69 |
| MOTA | 2822 | CA | ASP A 353 | | 67.337 | | 117.286 | 1.00 39.89 |
| ATOM | 2823 | CB | ASP A 353 | | | | | 1.00 43.53 |
| MOTA | 2824 | CG | ASP A 353 | | 65.058 | 15.368 | 116.211 | 1.00 47.99 |
| ATOM | 2825 | OD1 | ASP A 353 | | 64.253 | | 115.593 | 1.00 38.06 |
| ATOM | 2826 | OD2 | ASP A 353 | | 64.706 | | 116.898 | 1.00 52.94 |
| MOTA | 2827 | С | ASP A 353 | | 67.457 | 17.165 | 117.247 | 1.00 39.20 |
| MOTA | 2828 | 0 | ASP A 353 | | 66.890 | 17.861 | 118.092 | 1.00 35.66 |
| ATOM | 2829 | N | PRO A 354 | | 68.244 | 17.696 | 116.302 | 1.00 40.75 |
| ATOM | 2830 | CD | PRO A 354 | | 69.047 | 17.005 | 115.279 | 1.00 40.05 |
| ATOM | 2831 | CA | PRO A 354 | | 68.426 | 19.145 | 116.179 | 1.00 38.41 |
| ATOM | 2832 | CB | PRO A 354 | | 69.534 | | 115.140 | 1.00 36.24 |
| ATOM | 2833 | CG | PRO A 354 | | 69.190 | 18.095 | 114.225 | 1.00 39.41 |
| MOTA | 2834 | c | PRO A 354 | | 67.144 | 19.780 | 115.689 | 1.00 37.28 |
| ATOM | 2835 | 0 | PRO A 354 | | 66.299 | 19.106 | 115.094 | 1.00 31.87 |
| ATOM | 2836 | N | TRP A 355 | | 66.993 | 21.074 | 115.934 | 1.00 37.87 |
| ATOM | 2837 | CA | TRP A 355 | | 65.804 | 21.757 | 115.472 | 1.00 40.04 |
| ATOM | 2838 | CB | TRP A 355 | | 65.714 | 23.157 | 116.080 | 1.00 42.85 |
| WI OLD | | | | | | | | |

| | | • |
|--------------|--|--|
| MOTA | | 64.333 23.471 116.569 1.00 53.01 |
| ATOM | | 63.439 24.463 116.047 1.00 54.23 |
| ATOM | | 62.234 24.368 116.783 1.00.52.59 |
| ATOM | | 63.538 25.422 115.028 1.00 52.82 |
| ATOM | | 63.655 22.836 117.575 1.00 51.80 |
| ATOM ATOM | | 62.393 23.368 117.708 1.00 51.38 |
| ATOM | | 61.134 25.197 116.532 1.00 51.28 |
| ATOM | | 62.444 26.245 114.779 1.00 53.22 61.257 26.126 115.531 1.00 50 50 |
| ATOM | | |
| ATOM | | |
| ATOM | | 67.041 21.929 113.422 1.00 39.01 64.809 21.764 113.259 1.00 36.31 |
| MOTA | | 64.797 21.820 111.802 1.00 35.22 |
| ATOM | | 64.317 20.469 111.252 1.00 33.35 |
| MOTA | | 65.310 19.340 111.564 1.00 34.50 |
| ATOM | | 64.729 17.927 111.468 1.00 28.06 |
| MOTA | | 65.745 16.956 111.870 1.00 24.79 |
| MOTA MOTA | | 65.499 15.703 112.236 1.00 27.56 |
| ATOM | | 64.253 15.237 112.259 1.00 19.09 66.502 14.918 112.604 1.00 21 34 |
| ATOM | 2859 C ARG A 356 | (3 001 |
| ATOM | 2860 O ARG A 356 | 50 015 |
| MOTA | 2861 N GLY A 357 | 62.746 22.732 110.950 1.00 34.68 64.361 24.181 111.550 1.00 35.60 |
| ATOM | 2862 CA GLY A 357 | 63.556 25.345 111.220 1.00 35.43 |
| MOTA | 2863 C GLY A 357 | 63.719 25.932 109.830 1.00 38.08 |
| ATOM | 2864 O GLY A 357 | 64.112 25.250 108.885 1.00 37.29 |
| ATOM | 2865 N GLY A 358 2866 CA GLY A 358 | 63.406 27.218 109.721 1.00 39.67 |
| MOTA MOTA | 2866 CA GLY A 358 2867 C GLY A 358 | 63.493 27.925 108.457 1.00 36.36 |
| ATOM | 2868 O GLY A 358 | 62.398 28.966 108.499 1.00 39.45 61.763 29.131 109.539 1.00 37.58 |
| ATOM | 2869 N GLU A 359 | |
| ATOM | 2870 CA GLU A 359 | 62.163 29.662 107.391 1.00 40.89 61.121 30.682 107.358 1.00 41.37 |
| MOTA | 2871 CB GLU A 359 | 61.310 31.627 106.172 1.00 44.64 |
| MOTA | 2872 CG GLU A 359 | 60.956 30.977 104.848 1.00 52.13 |
| MOTA | . 2873 CD GLU A 359 | 60.833 31.973 103.708 1.00 59.14 |
| MOTA | 2874 OE1 GLU A 359 2875 OE2 GLU A 359 | 60.448 31.551 102.593 1.00 60.47 |
| ATOM ATOM | 2875 OE2 GLU A 359 2876 C GLU A 359 | 61.119 33.173 103.923 1.00 57.77 |
| ATOM | 2877 O GLU A 359 | 59.770 30.006 107.200 1.00 38.02 59.689 28.828 106.850 1.00 35.29 |
| ATOM | . 2878 N VAL A 360 | 2.00 33.25 |
| MOTA | 2879 CA VAL A 360 | 58.708 30.762 107.441 1.00 36.81 57.363 30.237 107.291 1.00 35.97 |
| ATOM | 2880 CB VAL A 360 | 56.401 30.789 108.368 1.00 34.90 |
| MOTA | 2881 CG1 VAL A 360 | 54.999 30.251 108.133 1.00 36.53 |
| ATOM | 2882 CG2 VAL A 360 | 56.888 30.393 109.755 1.00 37.06 |
| MOTA | 2883 C VAL A 360 2884 O VAL A 360 | 56.886 30.690 105.928 1.00 36.74 |
| ATOM ATOM | 2884 O' VAL A 360 2885 N ARG A 361 | 56.661 31.881 105.712 1.00 34.90 |
| ATOM | 2886 CA ARG A 361 | 56.753 29.741 105.004 1.00 35.48 56.301 30.049 103.652 1.00 38.21 |
| ATOM | 2887 CB ARG A 361 | 56.301 30.049 103.652 1.00 38.21 56.152 28.776 102.815 1.00 39.76 |
| ATCM | 2888 CG ARG A 361 | 57.416 28.342 102.098 1.00 39.93 |
| ATOM | 2889 CD ARG A 361 | 57.225 26.963 101.486 1.00 38.68 |
| ATCM | 2890 NE ARG A 361 | 57.112 25.940 102.525 1.00 39.72 |
| MOTA | 2891 CZ ARG A 361 | 56.952 24.643 102.286 1.00 38.79 |
| MOTA | 2892 NH1 ARG A 361 | 56.881 24.200 101.036 1.00 32.40 |
| ATOM | 2893 NH2 ARG A 361 2894 C ARG A 361 | 56.899 23.785 103.297 1.00 36.58 |
| ATOM ATOM | 2894 C ARG A 361 2895 O ARG A 361 | 54.996 30.807 103.603 1.00 38.98 |
| ATCM | 2896 N LYS A 362 | 54.120 30.636 104.452 1.00 39.07 54.880 31.634 102.573 1.00 39.95 |
| ATOM | 2897 CA LYS A 362 | 54.880 31.634 102.573 1.00 39.95 53.709 32.459 102.339 1.00 42.73 |
| ATCM | 2898 CB LYS A 362 | 53.931 33.301 101.078 1.00 44.92 |
| ATCH | 2899 CG LYS A 362 | 54.995 34.390 101.219 1.00 55.45 |
| atom | 2900 CD LYS A 362 | 56.351 33.842 101.671 1.00 58.28 |
| ATOM | 2901 CE LYS A 362 | 56.907 32.809 100.697 1.00 57.04 |
| HOTA | 2902 NZ LYS A 362 | 58.224 32.283 101.151 1.00 58.75 |
| ATOM | 2903 C LYS A 362 2904 O LYS A 362 | 52.434 31.634 102.200 1.00 40.51 |
| atch | 2709 U MIS A 302 | 51.391 31.996 102.748 1.00 36.10 |

Figure 18-45

| ATOM | 2905 | N | GLU 2 | A 363 | 52. | 506 30.52 | 7 101.469 | 1.00 | 37.79 |
|-------|------|-----|---------|-------|------|-----------|------------|------|-------|
| MOTA | 2906 | CA | GLU 2 | A 363 | 51.: | 313 29.70 | 5 101.295 | | 40.96 |
| ATOM | 2907 | | | A 363 | 51. | | 0 100.347 | | 43.62 |
| ATOM | 2908 | | | A 363 | 52. | | 6 100.739 | | 47.01 |
| ATOM | 2909 | | | A 363 | 52.9 | | | | 51.65 |
| ATOM | 2910 | | • | A 363 | 52.0 | | | | 45.63 |
| | 2910 | | | | | | | | |
| MOTA | | | | A 363 | 54.3 | | | | 48.44 |
| ATOM | 2912 | С | | A 363 | 50.1 | | 9 102.636 | | 37.74 |
| ATOM | 2913 | 0 | | 4.363 | 49.5 | | 3 102.834 | | 34.79 |
| ATOM | 2914 | N | | 364 | 51.6 | | .0 103.564 | | 33.64 |
| MOTA | 2915 | CA | VAL A | 364 | 51.2 | 274 28.45 | 5 104.886 | 1.00 | 32.39 |
| ATOM | 2916 | CB | | 364 | 52.4 | 184 28.04 | 8 105.749 | 1.00 | 33.99 |
| ATOM | 2917 | CG: | 1 VAL A | 364 | 52.0 | 18 27.67 | 6 107.160 | 1.00 | 36.90 |
| ATOM | 2918 | CG: | 2 VAL A | 364 | 53.3 | 198 26.86 | 7 105.109 | 1.00 | 29.56 |
| MOTA | 2919 | С | VAL A | 364 | 50.5 | 506 29.57 | 4 105.589 | 1.00 | 34.33 |
| MOTA | 2920 | 0 | VAL A | 364 | 49.4 | | 6 106.188 | | 29.80 |
| ATOM | 2921 | N | LYS A | | 51.0 | | | | 38.12 |
| ATOM | 2922 | CA | LYS A | | 50.3 | | | | 36.77 |
| ATOM | 2923 | CB | LYS A | | 51.2 | | | | 37.98 |
| MOTA | 2924 | CG | LYS A | | 52.6 | | | | 37.99 |
| ATOM | 2925 | CD | LYS A | | 53.4 | | | | 35.50 |
| | 2926 | CE | LYS A | | 54.8 | | | | 40.35 |
| ATOM | | | | | | | | | |
| MOTA | 2927 | ΝZ | LYS A | | 55.6 | | | | 43.74 |
| ATOM | 2928 | Ċ | LYS A | | 49.0 | | | | 36.62 |
| ATOM | 2929 | .0 | LYS A | | 48.0 | | | | 33.53 |
| MOTA | 2930 | N | ASP A | | 48.9 | • | | | 37.05 |
| MOTA | 2931 | CA | ASP A | | 47.7 | | 8 103.449 | | 37.72 |
| ATOM | 2932 | CB | ASP A | | 47.9 | | 7 101.929 | | 40.57 |
| ATOM | 2933 | CG | ASP A | | 48.8 | | | | 43.98 |
| MOTA | 2934 | ODI | | | 49.0 | | | | 38.51 |
| MOTA | 2935 | OD2 | ASP A | 366 | 49.2 | 97 33.23 | | | 41.96 |
| ATOM | 2936 | С | ASP A | 366 | 46.6 | | 8 103.862 | | 39.24 |
| ATOM | 2937 | 0 | ASP A | 366 | 45.4 | | 2.104.029 | | 39.04 |
| MOTA | 2938 | N | THR A | 367 | 47.0 | 96 29.99 | 0 104.031 | 1.00 | 38.99 |
| ATOM | 2939 | CA | THR A | 367 | 46.1 | 67 28.93 | 5 104.432 | 1.00 | 36.80 |
| ATOM | 2940 | CB | THR A | 367 | 46.8 | 68 27.56 | 0 104.527 | 1.00 | 33.84 |
| ATOM | 2941 | OG1 | THR A | 367 | 47.3 | 32 27.16 | 7 103.232 | 1.00 | 34.92 |
| ATOM | 2942 | CG2 | THR A | 367 | 45.9 | 04 26.50 | 9 105.046 | 1.00 | 35.11 |
| MOTA | 2943 | С | THR A | | 45.5 | | | | 36.58 |
| ATOM | 2944 | Ō | THR A | | 44.3 | | | | 30.18 |
| ATOM | 2945 | N | LEU A | | 46.3 | | | | 35.32 |
| ATOM | 2946 | CA | LEU A | | 45.8 | | | | 35.46 |
| ATOM | 2947 | CB | LEU A | | 46.9 | | 9 109.077 | | 34.03 |
| ATOM | 2948 | CG | LEU A | | 47.5 | | | | 39.04 |
| MOTA | 2949 | CD1 | | | 46.4 | | | | 37.35 |
| MOTA | 2950 | CD2 | | | 48.0 | | | | 39.52 |
| ATOM | 2951 | ·C | LEU A | | 44.9 | | 6 107.994 | | 38.12 |
| | 2952 | ō | LEU A | | 43.9 | | | | 31.70 |
| ATOM | | | GLU A | | | | 3 107.086 | | 40.45 |
| ATOM | 2953 | N | | | 45.3 | | 1 106.866 | | 45.36 |
| MOTA | 2954 | CA | GLU A | | 44.5 | | | | |
| ATOM | 2955 | CB | GLU A | | 45.1 | | 6 105.765 | | 47.38 |
| ATOM | 2956 | CG | GLU A | | 46.0 | | 8 106.283 | | 53.81 |
| ATOM | 2957 | CD | GLU A | | 45.2 | | 6 106.996 | | 59.97 |
| Mota | 2958 | OE1 | | | 45.8 | | 2 107.526 | | 60.65 |
| MOTA | 2959 | OE2 | | | 43.9 | | 1 107.016 | | 63.69 |
| MOTA | 2960 | С | GLU A | | 43.1 | | 5 106.466 | | 43.23 |
| ATOM | 2961 | 0 | GLU A | | 42.1 | | | | 44.62 |
| MOTA | 2962 | Ŋ | LYS A | | 42.9 | | | | 40.34 |
| ATOM | 2963 | CA | LYS A | | 41.6 | 66 31.63 | | 1.00 | 43.36 |
| ATOM | 2964 | CB | LYS A | | 41.7 | | | 1.00 | 44.79 |
| ATOM | 2965 | CG | LYS A | | 42.0 | 32 31.54 | 6 102.419 | 1.00 | 48.93 |
| ATOM | 2966 | CD | LYS A | | 43.5 | | 4 102.019 | | 51.41 |
| ATOM | 2967 | CE | LYS A | | 43.9 | | 6 101.561 | | 51.14 |
| ATOM | 2968 | NZ | LYS A | | 45.3 | | 2 101.091 | | 50.34 |
| MOTA | 2969 | С | LYS A | | 40.9 | 59 30.84 | B 106.069 | | 43.09 |
| ATOM | 2970 | ō | LYS A | | 39.7 | | 7 106.248 | | 41.34 |
| WI ON | | - | - | - | | | | | - |

Figure 18-46

| | | | • | | | |
|------|----------------|--------|------------------|----------------|------------------------|---------------------------------------|
| ATO | 1 2971 N ALA | A 371 | 41.719 | 5 30 03 | 7 100 00 | 2 2 00 5 |
| ATON | | A 371 | 41.120 | | 17 106.80 18 107.86 | |
| ATON | 1 2973 CB ALA | 371 | 42.193 | 2 2 2 4 4 | 0 107.86 | |
| ATON | 1 2974 C ALA | 371 | 40.365 | | 0 108.59 2 108.83 | |
| MOTA | 1 2975. O ALA | 371 | 39.230 | | | |
| ATOM | 1 2976 N LYS | | 40.981 | | 9 109.21 | |
| MOTA | | | 40.391 | | 9 109.22 | |
| ATOM | 2978 C LYS | 372 | 39.052 | | 8 110.19 | |
| ATOM | 2979 O LYS | 372 | 38.294 | | | |
| ATOM | 2980 CB LYS A | 372 | 41.334 | 33.31 | 8 110.43 | |
| ATOM | | | 42.804 | | | |
| ATOM | | | 43.746 | | 9 110.510 | |
| MOTA | | | | | 1 110.752 | |
| ATOM | | | 45.216 | | 5 110.849 | |
| ATOM | | | 46.121 | | 0 111.081 | |
| ATOM | | | 38.751 | | 6 108.397 | |
| ATOM | | | 37.492 | | 3 107.806 | |
| ATOM | 2988 C ALA A | 373 | 37.758 | 33.63 | 2 106.480 | |
| ATOM | 2989 O ALA A | | 36.524 | 31.77 | | |
| ATOM | 2990 OXT ALA A | | 35.432 | 31.797 | 7 108.205 | |
| ATOM | 3014 CB ALA B | 2 | 36.870 | 30.853 | 106.822 | |
| ATOM | 3015 C ALA B | | 54.881 | | | |
| MOTA | 3016 O ALA 9 | 2 | 53.960 | -2.137 | | |
| ATOM | 3017 N ALA B | 2 2 | 54.920 | -1.720 | | |
| ATOM | 3018 CA ALA B | | 54.263 | -3.672 | | |
| ATOM | 3019 N LYS B | 2 3 | 53.914 | -3.584 | | |
| ATOM | 3020 CA LYS B | 3 | 52.919 | -1.376 | | |
| MOTA | 3021 CB LYS B | 3 | 52.855 | 0.022 | | |
| MOTA | 3022 CG LYS B | 3 | 51.643 | 0.700 | | |
| ATOM | 3023 CD LYS 3 | 3 | 51.751 | 0.785 | | 1.00 53.37 |
| ATOM | 3024 CE LYS B | 3 | 50.685 | 1.681 | | 1.00 55.40 |
| MOTA | 3025 NZ LYS B | 3 | 50.808 | 1.783 | 52.277 | 1.00 59.51 |
| ATOM | 3026 C LYS B | 3 | 52.140 | 2.323 | 51.884 | 1.00 56.88 |
| ATOM | 3027 O LYS B | 3. | 52.849 | 0.238 | 58.059 | 1.00 46.83 |
| ATOM | 3028 N VAL B | . 4 | 52.389 53.376 | -0.607 | 58.830 | 1.00 41.63 |
| MOTA | 3029 CA VAL B | 4 | 53.483 | 1.385 | 58.467 | 1.00 41.46 |
| ATOM | 3030 CB VAL B | 4 | 54.893 | 1.751 | 59.871 | 1.00 40.85 |
| ATOM | 3031 CG1 VAL B | 4 | 55.070 | 2.288 2.541 | 60.163 | 1.00 39.55 |
| ATOM | 3032 CG2 VAL B | 4 | 55.916 | 1.306 | 61.648 | 1.00 41.23 |
| MOTA | 3033 C VAL B | 4 | 52.451 | 2.813 | 59.652 60.230 | 1.00 38.96 |
| ATOM | 3034 O VAL B | 4 | 52.472 | 3.916 | | 1.00 38.92 |
| MOTA | 3035 N LYS B | 5 | 51.559 | 2.479 | 59.691 61.157 | 1.00 42.80 |
| MOTA | 3036 CA LYS B | 5 | 50.501 | 3.396 | 61.558 | 1.00 34.90 |
| MOTA | 3037 CB LYS B | 5 | 49.133 | 2.796 | 61.215 | 1.00 31.22 |
| MOTA | 3038 CG LYS B | 5 | 48.841 | 2.623 | 59.726 | 1.00 33.76 |
| ATOM | 3039 CD LYS B | 5 | 48.667 | 3.964 | 59.032 | 1.00 36.60 |
| ATOM | 3040 CE LYS B | 5 | 48.234 | 3.803 | 57.577 | 1.00 41.48 |
| MOTA | 3041 NZ LYS B | 5 | 49.215 | 3.025 | 56.781 | 1.00 [.] 43.62 1.00 42.53 |
| MOTA | 3042 C LYS B | 5. | 50.512 | 3.749 | 63.038 | 1.00 42.53 |
| ATOM | 3043 O LYS B | 5 | 51.012 | 2.995 | 63.878 | 1.00 32.67 |
| MOTA | 3044 N LEU B | 6 | 49.937 | 4.906 | 63.343 | 1.00 25.78 |
| ATOM | 3045 CA LEU B | 6 | 49.821 | 5.379 | 64.712 | 1.00 27.07 |
| MOTA | 3046 CB LEU B | 6 | 50.596 | 6.696 | 64.896 | 1.00 31.09 |
| ATOM | 3047 CG LEU B | 6 | 50.691 | 7.340 | 66.285 | 1.00 30.13 |
| ATOM | 3048 CD1 LEU B | 6 | 49.333 | 7.827 | 66.728 | 1.00 28.09 |
| ATOM | 3049 CD2 LEU B | 6 | 51.248 | 6.338 | 67.282 | 1.00 38.87 |
| MOTA | 3050 C LEU B | 6 | 48.324 | 5.594 | 64.924 | 1.00 24.87 1.00 29.52 |
| MOTA | 3051. O LEU B | 6 | 47.669 | 6.287 | 64.149 | 1.00 29.52 |
| MOTA | 3052 N ILE B | 7 | 47.777 | 4.975 | 65.960 | 1 00 20 02 |
| MOTA | 3053 CA ILE B | 7 | 46.361 | 5.111 | 66.250 | 1.00 28.02 1.00 23.83 |
| MOTA | 3054 CB ILE B | 7 | 45.736 | 3.761 | 66.670 | |
| MOTA | 3055 CG2 ILE B | 7 | 44.309 | 3.974 | 67.127 | 1.00 25.11 1.00 23.59 |
| MOTA | 3056 CG1 ILE B | 7 | 45.690 | 2.794 | 65.477 | 1.00 23.39 |
| MOTA | 3057 CD1 ILE B | 7 | 47.021 | 2.406 | 64.906 | 1.00 31.00 |
| ATCM | 3058 C ILE B | 7 | 46.179 | 6.130 | 67.363 | 1.00 36.60 |
| MOTA | 3059 O ILE B | 7 | 46.766 | 6.005 | | 1.00 26.49 |
| | | | | 5.005 | | 1.00 40.00 |

| ATOM | 3060 | и с | GL | YE | 3 8 | 45.372 | 7.151 | 67.106 | 1 00 | 29.51 |
|--------------|--------------|------|------------|-----|----------|------------------|------------------|---------------------------------|------|-------|
| ATOM | 3061 | L CA | GL | Y E | 8 | 45.151 | | | | |
| MOTA | 3062 | ? C | GL | Y E | 8 | 44.217 | , | 67.667 | 1.00 | |
| ATOM | 3063 | | | YE | | 43.629 | | 66.590 | 1.00 | |
| ATOM | 3064 | l N | | R E | | 44.088 | | 68.509 | 1.00 | |
| ATOM- | 3065 | CA | | R E | | 43.234 | | 68.238 | | 29.37 |
| ATOM | 3066 | | | R B | | 41.748 | | 68.311 | | 32.64 |
| ATOM | 3067 | | | R B | | 40.959 | | 68.218 | | |
| ATOM | 3068 | | | R B | | 41.431 | | 69.637 | | 30.35 |
| ATOM | 3069 | | THI. | | | 43.479 | | | | 33.42 |
| ATOM | 3070 | | | RB | | 43.884 | | 69.302 | | 33.42 |
| MOTA | 3071 | | | JB | - | 43.228 | | 70.416 | | 30.46 |
| ATOM | 3072 | | LE | | 10 | 43.396 | 14.840 | 68.961 | | 32.05 |
| ATOM | 3073 | | LE | | 10 | 43.390 | 16.189 | 69. ⁻ 914- 69.190 | | 34.75 |
| ATOM | 3074 | | LE | | 10 | 44.605 | 16.578 | 68.355 | | 38.02 |
| ATOM | 3075 | | LEU | | 10 | 44.961 | 15.472 | | | 40.82 |
| ATOM | 3076 | | LEU | | 10 | | _ | 67.394 | | 43.62 |
| MOTA | 3077 | C. | LEU | | 10 | 44.314 | 17.869 | 67.605 | | 34.99 |
| ATOM | 3078 | | LEU | | 10 | 42.272 | 14.809 | 70.945 | | 34.25 |
| ATOM | 3078 | N | ASE | | 11 | 42.415 | 15.348 | 72.042 | | 33.13 |
| ATOM | 3080 | CA | ASF | | 11 | 41.158 | 14.169 | | | 30.61 |
| ATOM | 3081 | CB | ASF | | 11 | 40.011 | 14.098 | 71.501 | | 33.08 |
| ATOM | 3082 | CG | | | | 38.928 | 13.167 | 70.945 | | 37.57 |
| | 3083 | ODI | ASP ASP | | 11 | 38.372 | 13.643 | 69.621 | | 43.14 |
| MOTA | 3084 | OD2 | | | 11 | 38.013 | 14.834 | 69.525 | | 42.22 |
| ATOM | 3085 | C | ASP | | 11 | 38.281 | 12.825 | 68.681 | | 45.58 |
| MOTA | 3086 | ō | ASP | | 11 | 40.358 | 13.654 | 72.919 | | 32.19 |
| MOTA | 3087 | N | TYR | | 11 | 39.688 | 14.053 | 73.875 | | 23.44 |
| ATOM | 3088 | CA | TYR | | 12 | 41.386 | 12.822 | 73.066 | | 28.02 |
| ATOM ATOM | 3089 | CB | TYR | | 12 12 | 41.770 | 12.373 | 74.402 | | 32.00 |
| MOTA | 3090 | CG | TYR | | | 43.011 | 11.476 | 74.363 | | 28.67 |
| | 3091 | CD1 | | | 12 | 42.821 | 10.108 | 73.737 | | 25.33 |
| MOTA | 3092 | CE1 | | | 12 | 43.338 | 9.823 | 72.475 | | 23.74 |
| MOTA | 3093 | CD2 | | | 12 | 43.235 | 8.546. | 71.924 | | 22.85 |
| ATOM | 3094 | CE2 | | | 12 | 42.183 | 9.077 | 74.436 | | 21.93 |
| MOTA | 3095 | CZ | TYR | | 12 | 42.074 | 7.793 | 73.889 | | 21.99 |
| ATOM | 3096 | OH | TYR | | 12 | 42.605 | 7.538 | 72.640 | | 22.99 |
| MOTA | 3097 | C | TYR | | 12 | 42.532 | 6.273 | 72.109 | | 18.79 |
| MOTA | 3098 | Ö | TYR | | 12 12 | 42.054 | 13.567 | 75.319 | | 32.74 |
| MOTA MOTA | 3099 | N | GLY | | 13 | 41.986 | 13.450 | 76.542 | | 23.85 |
| ATOM | 3100 | CA | GLY | | 13 | 42.374 | 14.710 | 74.720 | | 26.96 |
| ATOM | 3101 | c | GLY | | 13 | 42.658 | 15.900 | 75.501 | | 34.92 |
| ATOM | 3102 | õ | GLY | | 13 | 41.452 41.580 | 16.396 | 76.277 | | 36.82 |
| ATOM | 3103 | N | LYS | | 14 | 40.279 | 17.228 15.875 | 77.176 | | 34.10 |
| ATOM | 3104 | CA | LYS | | 14 | 39.031 | 16.247 | 75.929 76.584 | | 37.23 |
| ATOM | 3105 | СВ | LYS | | 14 | 37.925 | 16.406 | 75.537 | | 41.77 |
| ATOM | 3106 | CG | LYS | | 14 | 38.110 | | | | 45.82 |
| ATOM | 3107 | CD | LYS | | 14 | 37.805 | 17.585 18.939 | 74.579 | | 51.38 |
| ATOM | 3108 | CE | LYS | | 14 | | | 75.241 | | 57.78 |
| ATOM | 3109 | NZ | LYS | | 14 | 38.752 38.387 | 19.285 | 76.388 77.070 | | 58.82 |
| | 3110 | C | LYS | | 14 | | 20.568 | | | 55.06 |
| ATOM | 3111 | ō | LYS | | 14 | 38.591 | 15.226 | 77.627 | | 39.50 |
| MOTA | 3112 | N | TYR | | 15 | 37.546 | 15.385 | 78.252 | | 35.54 |
| MOTA | 3113 | CA | TYR | | | 39.395 | 14.186 | 77.815 | | 40.97 |
| ATOM | 3114 | CB | TYR | | 15 | 39.070 | 13.128 | 78.768 | | 44.15 |
| ATOM | 3115 | CG | TYR | | 15 | 38.863 | 11.827 | 77.990 | | 44.42 |
| ATCM | | CD1 | TYR | | 15 | 37.850 | 11.972 | 76.876 | | 42.02 |
| ATOM | 3116 3117 | CE1 | TYR | | 15 | 38.064 | 11.389 | 75.634 | | 41.06 |
| ATOM | | | TYR | | 15 | 37.138 | 11.530 | 74.603 | 1.00 | |
| ATOM | 3118 | CD2 | | | 15 | 36.678 | 12.703 | 77.065 | | 42.99 |
| ATOM | 3119 | CE2 | TYR | | 15 | 35.748 | 12.851 | 76.048 | 1.00 | |
| ATOM | 3120 | CZ | TYR | | 15 | 35.984 | 12.261 | 74.816 | 1.00 | |
| ATCM | 3121 | | TYR | | 15 | 35.066 | 12.403 | 73.801 | 1.00 | |
| ATOM | 3122 | | TYR | | 15 | 40.151 | 12.944 | 79.838 | 1.00 | |
| ATOM | 3123 | | TYR | | 15 | 40.519 | 11.819 | 80.167 | 1.00 | |
| ATCM | 3124 | | ARG | | 16 | 40.647 | 14.052 | 80.381 | 1.00 | |
| atom | 3125 | CA . | ARG | ದ | 16 | 41.686 | 14.012 | 81.410 | 1.00 | 43.70 |

| ATO | M 3126 CB AF | RG B 16 | 42.2 | 50 15 41 | 0 02 55 | • |
|-------|----------------|----------------|--------|----------|----------------|--------------|
| ATO | | G B 16 | | | | |
| ATO | | | 42.6 | | 7 80.44 | 7 1.00 54.22 |
| | | G B 16 | 43.8 | 8 15.62 | 4 79.75 | 1 1.00 55.13 |
| ATON | | G B 16 | 44.30 | | | |
| ATOM | 1 3130 CZ AR | G B 16 | 44.62 | | | 42.07 |
| ATOM | | G B 16 | 44.02 | _ | | |
| ATOM | | 0 5 60 | 44.55 | | 8 80.18 | 2 1.00 65.86 |
| | | | 45.02 | 2 18.60 | 0 77.95 | 4 1.00 67.19 |
| ATOM | | G B 16 | 41.09 | | | |
| ATOM | 3134 O AR | G B 16 | | | | |
| ATOM | 2222 | | 39.88 | | | 7 1.00 38.44 |
| ATOM | | | 41.94 | 9 13.05 | 6 83.628 | 3 1.00 39.36 |
| | | R B 17 | 41.49 | 4, 12.63 | 7 84.949 | 1 00 37 67 |
| MOTA | 3137 CB TY | R B 17 | 42.50 | | | |
| ATOM | 3138 CG TY | R B 17 | | | _ | |
| MOTA | | | 42.41 | | 85.087 | 1.00 28.00 |
| ATOM | | R B 17 | .42.53 | 0 9.944 | 83.732 | 1.00 22.89 |
| | | R B 17 | 42.50 | 2 8.618 | | 1 00 21 40 |
| ATOM | 3141 CD2 TY | RB 17 | 42.25 | | | |
| ATOM | 3142 CE2 TYP | | | | | |
| ATOM | | | 42.22 | | | 1.00 24.48 |
| | | | 42.35 | 5 7.587 | 84.210 | 1.00 27.13 |
| MOTA | 3144 OH TYR | l B 17 | 42.37 | | | |
| ATOM | 3145 C TYR | B 17 | 41.37 | | | |
| ATOM | 3146 O TYR | | | | | |
| ATOM | | | 41.947 | | | 1.00 39.65 |
| | | | 40.647 | 7 13.893 | 86.891 | 1.00 41.27 |
| ATOM | 3148 CD PRO | B 18 | 39.958 | | 87.462 | |
| MOTA | 3149 CA PRO | B 18 | 40.448 | | | |
| ATOM | 3150 CB PRO | | | | 87.762 | |
| ATOM | | | 39.648 | | 88.928 | 1.00 44.09 |
| | | | 40.096 | 13.015 | 88.933 | 1.00 49.22 |
| ATOM | 3152 C PRO | B 18 | 41.702 | | 88.221 | 1 00 45 25 |
| MOTA | 3153 O PRO | B 18 | 42.789 | | | 1.00 45.86 |
| MOTA | 3154 N LYS | | | | 88.317 | 1.00 45.44 |
| MOTA | 3155 CA LYS | | 41.506 | | 88.507 | 1.00 48.42 |
| | | | 42.535 | 18.040 | 88.952 | 1.00 51.03 |
| ATOM | 3156 CB LYS | | 41.973 | 19.122 | 89.814 | 1.00 56.35 |
| ATOM | 3157 CG LYS | B 19 | 40.630 | | | 1.00 56.35 |
| ATOM | 3158 CD LYS | | | | 90.563 | 1.00 65.69 |
| ATOM | 3159 CE LYS | | 40.894 | 17.441 | 91.423 | 1.00 68.96 |
| | | — - | 39.602 | 16.882 | 91.999 | 1.00 71.85 |
| MOTA | 3160 NZ LYS | | 39.825 | 15.603 | 92.731 | 1.00 72.79 |
| ATOM | 3161 C LYS | B 19 | 43.830 | 17.593 | 89.639 | |
| Mota | 3162 O LYS | B 19 | | | | 1.00 48.62 |
| ATOM | 3163 N ASN | | 44.912 | 18.009 | 89.235 | 1.00 49.04 |
| ATOM | | | 43.745 | 16.775 | 90.678 | 1.00 43.99 |
| | | | 44.957 | 16.356 | 91.375 | 1.00 43.86 |
| ATOM | 3165 CB ASN | B 20 | 44.740 | 16.440 | 92.890 | 1.00 45.92 |
| ATOM | 3166 CG ASN | B 20 | 44.418 | | | 1.00 45.92 |
| ATOM | 3167 OD1 ASN | | | 17.848 | 93.355 | 1.00 49.44 |
| ATOM | | | 45.194 | 18.779 | 93.138 | 1.00 47.72 |
| | | | 43.268 | 18.011 | 93.999 | 1.00 49.42 |
| MOTA | 3169 C ASN 1 | | 45.460 | 14.960 | 91.008 | 1.00 39.49 |
| ATOM | 3170 O ASN 1 | B 20 | 46.496 | 14.521 | | 1.00 39.49 |
| MOTA | 3171 N HIS 1 | | | | 91.494 | 1.00 38.24 |
| ATOM | 3172 CA HIS I | | 44.729 | 14.274 | 90.140 | 1.00 36.93 |
| | | | 45.091 | 12.923 | 8 723 | 1.00 33.57 |
| ATOM | 3173 CB HIS I | | 43.948 | 12.299 | 87.924 | 1.00 28.67 |
| ATOM | 3174 CG HIS F | 3 21 | 44.068 | 10.817 | | 1.00 28.07 |
| ATOM | 3175 CD2 HIS E | | | | 88.750 | 1.00 32.14 |
| ATOM | 3176 ND1 HIS B | | 44.779 | 10.076 | 87.86 7 | 1.00 26.15 |
| | | | 43.431 | 9.917 | 89.578 | 1.00 29.59 |
| ATOM | 3177 CEI HIS E | 21 | 43.743 | 8.686 | 89.212 | 1.00 23.65 |
| ATCM | 3178 NE2 HIS B | 21 | 44.560 | 8.755 | 88.177 | 1.00 23.05 |
| ATOM | 3179 C HIS B | | 46.340 | | | 1.00 29.71 |
| | | | 46.348 | 12.928 | 88.852 | 1.00 29.06 |
| ATOM | | | 46.536 | 13.805 | 88.015 | 1.00 24.86 |
| ATCM | 3181 N PRO B | 22 | 47.225 | 11.937 | 89.035 | 1.00.30.50 |
| ATOM | 3182 CD PRO B | | 47.187 | 10.802 | | 1 00 35 5 |
| ATCM | 3183 CA PRO B | | | 10.802 | 89.976 | 1.00 31.51 |
| | | 22 | 48.446 | 11.880 | 88.231 | 1.00 29.58 |
| | | 22 | 49.055 | 10.549 | 88.656 | 1.00 33.72 |
| | 3185 CG PRO B | 22 | 43.658 | 10.489 | 90.124 | 1.00 31.07 |
| -TCM | 3186 C PRO B | 22 | 48.176 | | | 1.00 31.0/ |
| | 3187 O PRO B | | | | 86.728 | 1.00.28.52 |
| | | 22 | 48.989 | 12.474 | 85.972 | 1.00 31.85 |
| | | 23 | 47.030 | | | 1.00 24.47 |
| TCM . | 3189 CA LEU B | 23 | 46.685 | | 84.874 | 1.00 27.80 |
| TOM : | 3190 CB LEU B | 23 | 45.933 | | 04 E | 1.00 27.80 |
| | | | | | 84.513 | 1.00 22.18 |
| | 3191 CG LEU B | 23 | 46.760 | 8.852 | 84.556 | 1.00 29.32 |
| | | | | | | |

Figure 18-49

| | 2102 | cn1 | T 1771 D | 23 | 45.868 | 7.628 | 84.402 | 1.00 24.94 |
|--------|-------|-----|----------|----|----------|----------------|--------|------------|
| MOTA | 3192 | | LEU B | | | _ | 83.446 | 1.00 24.80 |
| ATOM | 3193 | CD2 | LEU B | 23 | 47.805 | 8.905 | | |
| ATOM | 3194 | С | LEU B | 23 | 45.891 | 12.638 | 84.367 | 1.00 27.95 |
| ATOM | 3195 | Э | LEU B | 23 | 45.166 | 12.528 | 83.373 | 1.00 24.42 |
| | | | LYS B | 24 | 46.011 | 13.793 | 85.018 | 1.00 31.01 |
| ATOM | 3196 | 71 | | | | | 84.530 | 1.00 29.40 |
| ATOM | 3197 | CA | LYS B | 24 | 45.261 | 14.946 | | |
| ATOM | 3198 | CB | LYS B | 24 | 44.934 | 15.923 | 85.665 | 1.00 33.03 |
| | 3199 | CG | LYS B | 24 | 45.979 | 16.969 | 85.999 | 1.00 33.54 |
| ATOM | | | | | 47.300 | 16.397 | 86.422 | 1.00 39.10 |
| MOTA | 3200 | CD | LYS B | 24 | | | | 1.00 45.49 |
| ATOM | 3201 | CE | LYS B | 24 | 48.109 | 17.466 | 87.152 | |
| ATOM | 3202 | NZ | LYS B | 24 | 48.224 | 18.737 | 86.380 | 1.00 45.95 |
| | 3203 | С | LYS B | 24 | 46.039 | 15.653 | 83.425 | 1.00 30.02 |
| ATOM | | | | | 45.508 | 16.523 | 82.736 | 1.00 28.82 |
| ATOM | 3204 | 0 | LYS B | 24 | | | | 1.00 25.93 |
| ATOM | 3205 | N | ILE B | 25 | 47.298 | 15.262 | 83.246 | |
| ATOM | 3206 | CA | ILE B | 25 | 48.139 | 15.858 | 82.212 | 1.00 29.48 |
| _ | 3207 | CB | ILE B | 25 | 49.641 | 15.528 | 82.409 | 1.00 33.61 |
| MOTA | | | | | 50.126 | 16.033 | 83.775 | 1.00 32.27 |
| MOTA | 3208 | CG2 | ILE B | 25 | | | 82.263 | 1.00 28.17 |
| ATOM | 3209 | CG1 | ILE B | 25 | 49.851 | 14.014 | | |
| ATOM | 3210 | CD1 | ILE B | 25 | 51.310 | 13.584 | 82.188 | 1.00 36.32 |
| ATOM | 3211 | С | ILE B | 25 | 47.784 | 15.318 | 80.834 | 1.00 30.08 |
| | | ō | ILE B | 25 | 47.263 | 14.210 | 80.704 | 1.00 25.37 |
| MOTA | 3212 | | | | | 16.101 | 79.783 | 1.00 29.19 |
| ATOM | 3213 | N | PRO B | 26 | 48.064 | | | 1.00 32.47 |
| ATOM | 3214 | CD | PRO B | 26 | 48.650 | 17.448 | 79.770 | • |
| ATOM | 3215 | CA | PRO B | 26 | 47.782 | 15.673 | 78.413 | 1.00 29.52 |
| | 3216 | CB | PRO B | 26 | 48.103 | 16.921 | 77.593 | 1.00 29.84 |
| MOTA | | | | | 47.930 | 18.046 | 78.599 | 1.00 36.40 |
| ATOM | 3217 | CG | PRO B | 26 | | | 78.137 | 1.00 27.64 |
| ATOM | 3218 | С | PRO B | 26 | 48.789 | 14.561 | | |
| ATOM | 3219 | 0 | PRO B | 26 | . 49.920 | 14.620 | 78.629 | 1.00 23.08 |
| ATOM | 3220 | N | ARG B | 27 | 48.403 | 13.557 | 77.360 | 1.00 23.09 |
| | 3221 | CA | ARG B | 27 | 49.326 | 12.469 | 77.072 | 1.00 23.00 |
| ATOM | | | | | | 11.264 | 77.962 | 1.00 26.21 |
| ATOM | 3222 | CB | ARG B | 27 | 48.987 | | 79.449 | 1.00 17.03 |
| MOTA | 3223 | CG | ARG B | 27 | 49.101 | 11.617 | | |
| ATOM | 3224 | CD | ARG B | 27 | 48.663 | 10.507 | 80.416 | 1.00 26.83 |
| | 3225 | NE | ARG B | 27 | 49.586 | 9.375 | 80.502 | 1.00 22.99 |
| ATOM | | | | 27 | 49.444 | 8.220 | 79.856 | 1.00 25.06 |
| MOTA | 3226 | CZ | ARG B | | | 8.022 | 79.059 | 1.00 17.74 |
| ATOM | 3227 | NH1 | | 27 | 48.408 | | | 1.00 23.38 |
| ATOM | 3228 | NH2 | ARG B | 27 | 50.336 | 7.253 | 80.027 | |
| MOTA | 3229 | С | ARG B | 27 | 49.329 | 12.097 | 75.595 | 1.00 22.54 |
| | 3230 | õ | ARG B | 27 | 50.214 | 12.526 | 74.852 | 1.00 21.86 |
| MOTA | | | | 28 | 48.352 | 11.318 | 75.148 | 1.00 20.64 |
| ATOM . | 3231 | И | VAL B | | | | 73.739 | 1.00 26.57 |
| MOTA | 3232 | CA | VAL B | 28 | 48.337 | 10.954 | | 1.00 30.92 |
| ATOM | 3233 | CB | VAL B | 28 | 47.242 | 9.917 | 73.424 | |
| ATOM | 3234 | CG1 | VAL B | 28 | 47.195 | 9.645 | 71.925 | 1.00 27.04 |
| | 3235 | CG2 | VAL B | 28 | 47.535 | 8.616 | 74.172 | 1.00 25.45 |
| ATOM | | | | | 48.150 | 12.189 | 72.866 | 1.00 28.02 |
| ATOM | 3236 | С | VAL B | 28 | | | | 1.00 30.88 |
| ATOM | 3:37 | J | VAL B | 28 | 48.780 | 12.311 | 71.808 | |
| ATOM | 3.38 | N | SER B | 29 | 47.298 | 13.112 | 73.304 | 1.00 24.30 |
| | 3139 | CA | SER B | 29 | 47.082 | 14.326 | 72.523 | 1.00 29.48 |
| ATOM | | | SER B | 29 | 45.939 | 15.169 | 73.110 | 1.00 31.72 |
| MOTA | 3240 | CB | | | | 15.614 | 74.424 | 1.00 34.55 |
| ATOM | 3241 | OG | SER B | 29 | 46.218 | 13.014 | 72.514 | |
| ATOM | 3242 | C | SER B | 29 | 48.379 | 15.125 | | |
| ATOM | 3243 | Э | SER B | 29 | 48.680 | 15.820 | 71.545 | 1.00 28.85 |
| - | | IJ | LEU B | | 49.157 | 15.003 | 73.589 | 1.00 29.63 |
| MOTA | 3244 | | | | | 15.721 | 73.679 | 1.00 31.59 |
| ATOM | .3245 | CA | LEU B | 30 | 50.427 | 15.721 | | 1.00 29.49 |
| ATOM | 3246 | CB | LEU B | 30 | 51.046 | 15.593 | 75.079 | |
| ATOM | 3247 | CG | LEU B | 30 | 52.066 | 16.660 | 75.513 | 1.00 34.37 |
| | 3248 | | LEU B | 30 | 52.937 | 16.083 | 76.610 | 1.00 30.15 |
| ATOM | | | | | 52.951 | 17.098 | 74.357 | 1.00 32.90 |
| ATOM | 3249 | | LEU B | 30 | | | | 1.00-25.90 |
| ATOM | 3250 | C | LEU B | 30 | 51.371 | 15.085 | 72.672 | |
| ATOM | 3251 | Э | LEU B | 30 | 52.052 | 15.777 | 71.913 | 1.00 25.10 |
| | 3252 | N | LEU B | 31 | 51.404 | <u>1</u> 3.756 | 72.675 | 1.00 22.10 |
| atom | | | | | 52.268 | 13.013 | 71.764 | 1.00 25.52 |
| ATOM | 3253 | CA | LEU B | | | 11 614 | 71.842 | 1.00 26.41 |
| MOTA | 3254 | CB | LEU B | | 51.966 | 11.514 | | 1.00 20.41 |
| ATOM | 3255 | CG | LEU B | 31 | 53.066 | 10.524 | 71.441 | 1.00 28.93 |
| | 3256 | | LEU B | | 52.425 | 9.198 | 71.042 | 1.00 23.69 |
| ATOM | | | | | 53.873 | 11.049 | 70.300 | 1.00 30.41 |
| ATOM | 3257 | CDZ | LEU B | 71 | 23.072 | 11.0 | _ | |
| | | | | | | | | |

| MOTA | 3258 | С | LEU | כו | 31 | | E2 010 | 33 400 | 70 775 | 1 00 05 34 |
|------|--------|-----|-------|----|------|---|-----------------|--------|--------|------------|
| | | | LEU | | | | 52.010 | 13.489 | 70.335 | 1.00 25.38 |
| MOTA | 3259 | | | | 31 | | 52.940 | 13.851 | 69.614 | 1.00 21.0 |
| MOTA | 3260 | N | LEU | | 32 | | 50.741 | 13.481 | 69.933 | 1.00 21.2 |
| ATOM | 3261 | CA | LEU | | 32 | | 50.364 | 13.899 | 68.585 | 1.00 27.91 |
| ATOM | 3262 | CB | LEU | | 32 | | 48.841 | 13.798 | 68.408 | 1.00 26.60 |
| ATOM | 3263 | CG | LEU | | 32 | | 48.195 | 12.419 | 68.614 | 1.00 27.30 |
| MOTA | 3264 | | 1.LEU | | 32 | | 46.699 | 12.504 | 68.321 | 1.00 31.60 |
| MOTA | 3265 | CD: | 2 LEU | 3 | 32 | | 48.837 | 11.391 | 67.708 | 1.00 26.90 |
| ATOM | 3266 | С | LEU | 3 | . 32 | | 50.835 | 15.317 | 68.242 | 1.00 26.07 |
| ATOM | 3267 | 0 | LEU | 3 | 32 | | 51.458 | 15.533 | 67.205 | 1.00 22.45 |
| ATOM | 3268 | N | ARG | В | 33 | - | 50.545 | 16.282 | 69.111 | 1.00 28.19 |
| ATOM | 3269 | CA | ARG | 3 | 33 | | 50.962 | 17.660 | 68.865 | 1.00 31.77 |
| ATOM | 3270 | CB | ARG | | 33 | | 50.395 | 18.601 | 69.930 | 1.00 34.22 |
| ATOM | 3271 | CG | ARG | | 33 | | 48.887 | 18.740 | 69.904 | 1.00 40.33 |
| ATOM | 3272 | CD | ARG | | 33 | | 48.420 | 19.713 | 70.970 | 1.00 47.67 |
| ATOM | 3273 | NE | ARG | | 33 | | 46.977 | 19.931 | 70.924 | 1.00 56.24 |
| ATOM | 3274 | CZ | ARG | | 33 | | 46.330 | 20.505 | 69.912 | 1.00 60.10 |
| ATOM | 3275 | NH: | | | 33 | | 46.997 | 20.929 | 68.845 | 1.00 63.11 |
| ATOM | 3276 | NH2 | | | 33 | | 45.011 | 20.652 | 69.965 | |
| | 3277 | C | ARG | | 33 | | | | | 1.00 63.81 |
| MOTA | 3278 | Ö | | | | | 52.476 | 17.791 | 68.852 | 1.00 30.12 |
| MOTA | 3279 | | ARG | | 33 | | 53.028 | 18.580 | 68.097 | 1.00 30.20 |
| MOTA | | N | PHE | | 34 | | 53.147 | 17.012 | 69.694 | 1.00 30.70 |
| ATOM | 3280 | CA | PHE | | 34 | | 54.600 | 17.060 | 69.774 | 1.00 29.42 |
| MOTA | 3281 | CB | PHE | | 34 | | 55.096 | 16.176 | 70.920 | 1.00 30.46 |
| ATOM | 3282 | CG | PHE | | 34 | | 56.556 | 16.358 | 71.248 | 1.00 28.56 |
| MOTA | 3283 | CD1 | | | 34 | | 57.001 | 17.515 | 71.885 | 1.00 26.92 |
| MOTA | 3284 | CD2 | | 3 | 34 | | 57.481 | 15.373 | 70.932 | 1.00 28.88 |
| ATOM | 3285 | CE1 | | 2 | 34 | | 58.346 | 17.684 | 72.206 | 1.00 28.15 |
| ATOM | 3286 | CE2 | | 3 | 34 | | 58.831 | 15.530 | 71.246 | 1.00 31.47 |
| MOTA | 3287 | CZ | PHE | | 34 | | 59.265 | 16.689 | 71.887 | 1.00 28.15 |
| MOTA | 3288 | С | PHE | | 34 | | 55.202 | 16.583 | 68.460 | 1.00 33.78 |
| ATOM | 3289 | 0 | PHE | | 34 | | 56.049 | 17.259 | 67.873 | 1.00 33.71 |
| MOTA | 3290 | N | LYS | | 35 | | 54.770 | 15.413 | 67.999 | 1.00 28.65 |
| MOTA | 3291 | CA | LYS | В | 3,5 | | 55.294 | 14.880 | 66.753 | 1.00 34.33 |
| MOTA | 3292 | CB | | В | 35 | | 54.684 | 13.509 | 66.454 | 1.00 32.97 |
| MOTA | 3293 | CG | LYS | | 35 | | 55.141 | 12.423 | 67.414 | 1.00 34.93 |
| MOTA | 3294 | CD | LYS | В | 35 | | 54.580 | 11.066 | 67.047 | 1.00 41.43 |
| MOTA | 3295 | CE | LYS | В | 35 | | 53.070 | 11.004 | 67.205 | 1.00 44.04 |
| ATOM | 3296 | NZ | LYS | 3 | 35 | • | 52.335 | 11.984 | 66.345 | 1.00 60.09 |
| atom | 3297 | С | LYS | В | 35 | | 5 5.01 5 | 15.842 | 65.608 | 1.00 35.78 |
| MOTA | 3298 | 0 | LYS | 3 | 35 | | 55.869 | 16.061 | 64.752 | 1.00 33.39 |
| ATOM | 3299 | H | ASP | В | 36 | | 53.823 | 16.426 | 65.602 | 1.00 32.32 |
| ATOM | 3300 | CA | ASP | 3 | 36 | | 53.468 | 17.365 | 64.552 | 1.00 36.31 |
| ATOM | . 3301 | CB | ASP | 3 | 36 | | 52.015 | 17.800 | 64.698 | 1.00 42.56 |
| ATOM | 3302 | CG | ASP | 3 | 36 | | 51.617 | 18.822 | 63.661 | 1.00 43.03 |
| MOTA | 3303 | OD1 | ASP | 3 | 36 | | 51.812 | 18.544 | 62.461 | 1.00 °9.17 |
| ATOM | 3304 | OD2 | ASP | В | 36 | | 51.111 | 19.897 | 64.043 | 1.00 .4.34 |
| ATOM | 3305 | С | ASP | В | 36 | | 54.371 | 18.590 | 64.578 | 1.00 '6.14 |
| ATOM | 3306 | 0 | ASP | 3 | 36 | | 54.764 | 19.099 | 63.534 | 1.00 32.40 |
| ATOM | 3307 | N | ALA | В. | 37 | | 54.694 | 19.061 | 65.777 | 1.00 34.80 |
| ATOM | 3308 | CA | ALA | В | 37 | | 55.554 | 20.226 | 65.924 | 1.00 36.82 |
| ATOM | 3309 | CB | ALA | В | 37 | | 55.599 | 20.659 | 67.383 | 1.00 38.54 |
| MOTA | 3310 | c | ALA : | | 37 | | 56.959 | 19.901 | 65.429 | 1.00 37.66 |
| ATOM | 3311 | 0 | ALA : | | 37 | | 57.675 | 20.776 | 64.950 | 1.00 30.56 |
| ATOM | 3312 | N | MET : | | 38 | | 57.346 | 18.635 | 65.541 | 1.00 37.42 |
| MOTA | 3313 | CA | HET : | | 38 | | 58.670 | 18.192 | 65.107 | 1.00 36.25 |
| ATOM | 3314 | CB | | 3 | 38 | | 59.158 | 17.059 | 66.013 | 1.00 36.44 |
| ATOM | 3315 | CG | MET | | 38 | | 59.341 | 17.438 | 67.474 | 1.00 37.68 |
| ATOM | 3316 | SD | MET | | 38 | | 60.841 | 18.391 | 67.784 | 1.00 38.07 |
| ATOM | 3317 | CE | MET : | | 38 | | 62.093 | 17.228 | 67.300 | 1.00 30.98 |
| ATOM | 3318 | c | MET ! | | 38 | | 58.639 | 17.690 | 63.663 | 1.00 35.86 |
| ATOM | 3319 | ō | MET | | 38 | | 59.659 | 17.262 | 63.130 | 1.00 32.69 |
| ATOM | 3320 | N | ASN I | | 39 | | 57.470 | 17.742 | 63.035 | 1.00 35.82 |
| ATOM | 3321 | CA | ASN I | | 39 | | 57.321 | 17.742 | 61.661 | 1.00 42.75 |
| ATOM | 3322 | CB | ASN I | | 39 | | 58.156 | 18.108 | 60.688 | 1.00 46.20 |
| ATOM | 3323 | CG | ASN I | | 39 | | 57.670 | 19.543 | 60.591 | 1.00 47.57 |
| ALUM | 23 | | I | - | | | 5 | | | |



| | | | | | | | _ | | | | |
|--------------|--------------|----------|------------|----|----------|---|------------------|----------------|------------------|------|----------------|
| ATOM | 3324 | OD | 1 ASI | ΙВ | 39 | | 56.524 | 19.801 | 60.212 | 1.00 | 48.78 |
| ATOM | 3325 | | 2 ASI | | 39 | | 58.540 | 20.486 | 60.933 | 1.00 | |
| ATOM | 3326 | С | ASI | | 39 | | 57.759 | 15.804 | 61.569 | 1.00 | |
| MOTA | 3327 | 0 | ASI | | 39 | | 58.465 | 15.416 | 60.639 | 1.00 | |
| ATOM | 3328 | N | LE | | 40 | | 57.332 | 14.997 | 62.535 | 1.00 | |
| ATOM | 3329 | CA | LE | | 40 | | 57.700 | 13.590 | 62.556 | 1.00 | |
| ATOM | 3330 | CB | LE | | 40 | | 58.347 | 13.248 | 63.898 | 1.00 | - |
| ATOM | 3331 | CG | LEU | | 40 | | 59.595 | 14.073 | 64.227 | 1.00 | |
| ATOM | 3332 | | 1 LEU | | 40 | | 60.148 | 13.648 | 65.573 | 1.00 | 36.57 |
| ATOM | 3333 | | 2 - LEU | | 40 | | 60.646 | 13.880 | 63.145 | 1.00 | |
| MOTA | 3334 | c c | LEU | | 40 | | 56.549 | 12.626 | 62.264 | 1.00 | 37.58 |
| ATOM | 3335 | ŏ | LEU | | 40 | | 56.637 | 11.438 | 62.573 | 1.00 | |
| ATOM | 3336 | N | ILE | | 41 | | 55.476 | 13.131 | 61.663 | 1.00 | |
| MOTA | 3337 | CA | ILE | | 41 | | 54.340 | 12.290 | 61.314 | 1.00 | |
| ATOM | 3338 | CB | ILE | | 41 | | 53.445 | 11.991 | 62.536 | 1.00 | 35.21 |
| ATOM | 3339 | CG2 | | | 41 | | 52.793 | 13.271 | 63.047 | 1.00 | 31.89 |
| ATOM | 3340 | CG1 | | | 41 | | 52.367 | 10.980 | 62.141 | 1.00 | 32.68 |
| ATOM | 3341 | CDI | | | 41 | | 51.470 | 10.550 | 63.285 | 1.00 | 36.46 |
| ATOM | 3342 | С | ILE | | 41 | | 53.492 | 12.937 | 60.229 | 1.00 | 37.52 |
| ATOM | 3343 | 0 | ILE | | 41 | | 53.352 | 14.157 | 60.183 | 1.00 | 40.24 |
| MOTA | 3344 | N | ASP | | 42 | | 52.943 | 12.114 | 59.345 | 1.00 | 39.55 |
| ATOM | 3345 | CA | ASP | В | 42 | | 52.094 | 12.615 | 58.273 | 1.00 | |
| MOTA | 3346 | CB | ASP | В | 42 | | 52.569 | 12.119 | 56.901 | | 45.93 |
| MOTA | 3347 | CG | ASP | В | 42 | | 53.972 | 12,584 | 56.564 | 1.00 | 47.09 |
| ATOM | 3348 | OD1 | ASP | В | 42 | | 54.244 | 13.799 | 56.686 | 1.00 | 46.60 |
| ATOM | 3349 | OD2 | ASP | В | 42 | | 54.797 | 11.736 | 56.162 | 1.00 | 45.16 |
| ATOM | 3350 | С | ÄSP | В | 42 | | 50.677 | 12.134 | 58.524 | 1.00 | 45.15 |
| ATOM | 3351 | 0 | ASP | В | 42 | | 50.467 | 11.051 | 59.069 | 1.00 | 47.06 |
| ATCM | 3352 | N | GLU | В | 43 | | 49.707 | 12.944 | 58.121 | 1.00 | 48.13 |
| MOTA | 3353 | CA | GLU | | 43 | | 48.303 | 12.618 | 58.312 | | 50.50 |
| MOTA | 3354 | CB | GLU | | 43 | | 47.441 | 13.637 | 57.57 1 | 1.00 | 53.54 |
| MOTA | 3355 | CG | GLU | | 43 | | 45.961 | 13.505 | 57.840 | 1.00 | 59.52 |
| MOTA | 3356 | CD | GLU | | 43 | | 45.155 | 14.518 | 57.065 | | 64.03 |
| MOTA | 3357 | OE1 | | | | • | 43.914 | 14.535 | 57.215 | 1.00 | 68.54 |
| MOTA | 3358 | OE2 | | | 43 | | 45.765 | 15.298 | 56.301 | 1.00 | 66.95 |
| MOTA | 3359 | C | GLU | | 43 | | 47.972 | 11.205 | 57.836 | 1.00 | 47.81 |
| MOTA | 3360 | 0 | GLU | | 43 | | 47.092 | 10.547 | 58.390 | | 49.67 |
| ATOM | 3361 | N | LYS | | 44 | | 48.690 | 10.744 | 56.817 | | 46.21 |
| ATOM | 3362 3363 | CA CB | LYS | | 44 | | 48.484 | 9.409 | 56.251 | | 48.28 |
| MOTA MOTA | 3364 | CG | LYS LYS | | 44 44 | | 49.207 49.639 | 9.311 7.903 | 54.894 54.470 | | 49.96 52.18 |
| MOTA | 3365 | CD | LYS | | 44 | | 50.970 | 7.532 | 55.127 | | 61.03 |
| ATOM | 3366 | CE | LYS | | 44 | | 51.399 | 6.095 | 54.844 | | 62.80 |
| ATOM | 3367 | NZ | LYS | | 44 | | 50.511 | 5.098 | 55.510 | | 65.34 |
| ATOM | 3368 | C | LYS | | 44 | | 48.899 | 8.249 | 57.161 | | 45.92 |
| ATOM | 3369 | ō | LYS | | 44 | | 48.418 | 7.127 | 57.009 | | 41.30 |
| ATOM | 3370 | N | GLU | | 45 | | 49.797 | 8.517 | 58.100 | | 42.18 |
| ATOM | 3371 | CA | GLU | | 45 | | 50.268 | 7.486 | 59.014 | | 38.41 |
| ATOM | 3372 | CB | GLU | | 45 | | 51.684 | 7.812 | 59.468 | | 33.73 |
| ATOM | 3373 | CG | GLU | | 45 | | 52.694 | 7.887 | 58.351 | | 37.58 |
| ATOM | 3374 | | GLU | | 45 | | 53.998 | 8.504 | 58.813 | | 34.34 |
| ATOM | 3375 | | GLU | | 45 | | 53.997 | 9.699 | 59.176 | | 38.04 |
| MOTA | 3376 | | GLU | | 45 | | 55.020 | 7.799 | 58.821 | 1.00 | 33.37 |
| MOTA | 3377 | С | GLU | В | 45 | | 49.368 | 7.403 | 60.238 | 1.00 | 36.86 |
| ATOM | 3378 | 0 | GLU | В | 45 | | 49.461 | 6.462 | 61.032 | 1.00 | 34.98 |
| ATCM | 3379 | N | LEU | В | 46 | | 48.489 | 8.386 | 60.386 | 1.00 | 30.86 |
| MOTA | 3380 | CA | LEU | В | 46 | | 47.608 | 8.438 | 61.545 | 1.00 | 30.65 |
| Mota | 3381 | CE | LEU | В | 46 | | 47.501 | 9.889 | 62.019 | | 32.74 |
| MOTA | 3382 | CG | LEU | В | 46 | | 46.642 | 10.163 | 63.250 | | 34.76 |
| MOTA | 3383 | CD1 | LEU | В | 46 | | 47.189 | 9.379 | 64.425 | | 32.24 |
| MOTA | 3384 | CD2 | LEU | В | 46 | | 46.639 | 11.656 | 63.548 | | 33.94 |
| ATOM | 3385 | C | LEU | | 46 | | 46.212 | 7.861 | 61.318 | | 31.36 |
| ATOM | 3386 | | LEU | | 46 | | 45.530 | 8.218 | 60.363 | | 31.78 |
| ATOM | 3387 | N | ILE | | 47 | | 45.801 | 5.957 | 62.203 | | 31.18 |
| ATCM | 3388 | CA | ILE | | 47 | | 44.479 | 6.338 | 62.139 | | 29.36 |
| ATOM | 3389 | CB | ILE | В | 47 | | 44.564 | 4.802 | 62.258 | 1.00 | 28.62 |

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Figure 18-52

| ATOM | 339 | 000 | | | | | | | |
|--------|------|------------|----------|---|----------|----------|--------|--------|---------|
| | | | | | 43.16 | 1 4.205 | 62.40 | 7 1.00 | 0 28.80 |
| ATOM | | | EB 47 | | 45.26 | 6 4.230 | 61.028 | | 0 29.42 |
| ATOM | 339 | 32 CD1 ILE | EB 47 | | 45.41 | | | | 0 31.12 |
| ATOM | 339 | 3 C ILE | | | 43.65 | | | | |
| ATOM | | | | | | | | | 32.22 |
| | | | | | 44.06 | | 64.461 | 1.00 | 31.17 |
| ATOM | | | | | 42.51 | 4 7.475 | 62.999 | | 28.39 |
| MOTA | 339 | 6 CA LYS | B 48 | | 41.66 | | | | 32.37 |
| ATOM | 339 | | | | 40.51 | | | | |
| MOTA | 339 | | | | | | | | 36.32 |
| ATOM | | | | | 39.60 | | | 1.00 | 43.08 |
| | | _ | | | 38.53 | 5 10.361 | 63.747 | 1:00 | 44.38 |
| MOTA | | | B 48 | - | 37.657 | 7 11.074 | 64.768 | 1.00 | 45.91 |
| ATOM | 340 | 1 NZ LYS | B 48 | | 38.451 | | | | 42.66 |
| . ATOM | 340 | 2 C LYS | B 48 | | 41.095 | | | 1.00 | 42.00 |
| ATOM | 340 | | | | | | | 1.00 | 31.08 |
| ATOM | 340 | | | | 40.524 | | | -1.00 | 26.24 |
| | | | • | | 41.260 | | 66.244 | 1.00 | 27.89 |
| ATOM | 340 | _ | | | 40.770 | 6.168 | 67.232 | | 25.17 |
| MOTA | 340 | 6 CB SER | B 49 | | 41.146 | 6.639 | | | 24.41 |
| MOTA | 340 | 7 OG SER | B 49 | | 42.539 | | 68.777 | 1.00 | 23.47 |
| MOTA | 340 | | | | | | | 1.00 | 31.79 |
| ATOM | 340 | | | | 39.248 | | 67.160 | | 29.07 |
| | | _ | | | 38.565 | 7.034 | 66.879 | 1.00 | 28.47 |
| MOTA | 3410 | | B 50 | | 38.723 | 4.859 | 67.409 | 1.00 | 26.13 |
| ATOM | 3413 | l CA ARG | B 50 | | 37.278 | | 67.430 | | 24.24 |
| ATOM | 3412 | CB ARG | B 50 | | 36.810 | | | | |
| ATOM | 3413 | | | | | | 66.323 | 1.00 | 25.03 |
| ATOM | 3414 | | | | 37.231 | | 66.507 | | 26.54 |
| | | | | | 36.570 | | 65.452 | 1.00 | 26.21 |
| ATOM | 3415 | _ | | | 37.006 | -0.058 | 65.504 | | 25.13 |
| ATOM | 3416 | CZ ARG | B 50 | | 36.700 | -0.924 | 66.468 | | 26.09 |
| MOTA | 3417 | NH1 ARG | B 50 | | 35.941 | -0.558 | 67.497 | | 23.42 |
| MOTA | 3418 | NH2 ARG | | | 37.157 | -2.168 | | | |
| ATOM | 3419 | | | | | | 66.402 | | 23.91 |
| ATOM | 3420 | | | | 36.937 | 4.037 | 68.775 | | 23.83 |
| | | | | | 37.782 | 3.392 | 69.403 | 1.00 | 21.60 |
| MOTA | 3421 | | B 51 | | . 35.700 | 4.223 | 69.243 | | 22.99 |
| MOTA | 3422 | CD PRO | B 51 | | 34.554 | 4.962 | | | 25.09 |
| ATOM | 3423 | ÇA PRO | B 51 | | 35.338 | 3.628 | 70.530 | 1.00 | |
| ATOM | 3424 | CB PRO | B 51 | | 33.949 | 4.217 | 70.802 | | 26.32 |
| ATOM | 3425 | CG PRO | | | 33.936 | | | | |
| MOTA | 3426 | C PRO | | | | 5.503 | 69.953 | 1.00 | 28.65 |
| ATOM | 3427 | | | | 35.264 | 2.118 | 70.325 | 1.00 | 26.73 |
| | | | | | 35.142 | 1.646 | 69.194 | 1.00 | 18.87 |
| ATOM | 3428 | N ALA | | | 35.355 | 1.359 | 71.408 | 1.00 | 23.64 |
| ATOM | 3429 | CA ALA | | | 35.237 | -0.083 | 71.291 | 1.00 | 23.27 |
| MOTA | 3430 | CB ALA | B 52 | | 35.811 | -0.757 | 72.521 | 1.00 | 26.31 |
| ATOM | 3431 | C ALA I | B 52 | | 33.733 | -0.324 | 71.223 | | 25.25 |
| ATOM | 3432 | O ALA | | | | | | | |
| ATOM | 3433 | N THR | | | 32.950 | 0.515 | 71.677 | 1.00 | 22.78 |
| ATOM | 3434 | | | | 33.321 | -1.447 | 70.651 | | 22.77 |
| | | - | | | 31.900 | -1.760 | 70.596 | 1.00 | 26.90 |
| ATOM | 3435 | CB THR E | | | 31.567 | -2.732 | 69.456 | 1.00 | 30.00 |
| MOTA | 3436 | OG1 THR E | | | 32.305 | -3.950 | 69.642 | 1.00 | 25.59 |
| ATOM | 3437 | CG2 THR E | 3 53 | | 31.917 | -2.117 | 68.103 | | 23.33 |
| MOTA | 3438 | C THR B | 53 | | 31.579 | -2.445 | 71.916 | | |
| ATOM | 3439 | O THR B | | | | | | | 30.41 |
| MOTA | 3440 | N LYS B | | | 32.484 | -2.917 | 72.609 | | |
| | | | | | 30.300 | -2.504 | 72.268 | 1.00 | 29.12 |
| ATOM | 3441 | CA LYS B | | | 29.909 | -3.140 | 73.514 | .1.00 | 30.24 |
| MOTA | 3442 | CB LYS B | | | 28.396 | -3.027 | 73.720 | | 32.78 |
| MOTA | 3443 | CG LYS B | 54 | | 27.947 | -3.351 | 75.131 | 1 00 | 34.85 |
| ATOM | 3444 | CD LYS B | | | 26.445 | | 75.268 | | |
| ATOM | 3445 | CE LYS B | | | 26 000 | -3.204 | 76 700 | 1.00 | 41.13 |
| | 3446 | NZ LYS B | 5 A | | 26.008 | -3.366 | 76.709 | 1.00 | |
| ATOM | | | | | 26.464 | -2.257 | 77.582 | 1.00 | 47.39 |
| ATOM | 3447 | C LYS B | 54 | | 30.329 | -4.603 | 73.442 | 1.00 | 29.10 |
| ATOM | 3448 | O LYS B | 54 | | 30.779. | -5.183 | 74.430 | 1.00 | |
| ATOM | 3449 | N GLU B | 55 | | 30.196 | -5.187 | 72.256 | 1.00 | |
| ATOM | 3450 | CA GLU B | 55 | | 30.577 | -6.577 | 72.032 | | 28.08 |
| ATCM | 3451 | CB GLU B | 55 | | 30.288 | -6.965 | 70.579 | | |
| ATOM | 3452 | CG GLU B | 55 | | | | | 1:00 | |
| | | | | | 30.671 | -8.400 | 70.237 | | 33.40 |
| ATOM | 3453 | CD GLU B | 55 75 | | 30.453 | -8.737 | 68.767 | | 38.49 |
| ATOM | 3454 | OE1 GLU B | 55 | | 30.638 | -9.913 | 68.394 | 1.00 | 41.24 |
| ATOM | 3455 | OE2 GLU 5 | 55 | 3 | 30.101 | -7.833 | 67.984 | 1.00 | 40.02 |
| | | | | | | | | | |

ATCM

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```
72.345
                                                              1.00 25.82
                                            -6.808
                                   32.066
                   GLU B
                           55
MOTA
        3456
               C
                                            -7.765
                                                     73.033
                                                              1.00 23.83
        3457
               O
                   GLU B
                           55
                                   32.429
ATOM
                                                              1.00 25.04
                                   32.931
                                            -5.938
                                                     71.835
MOTA
        3458
               N
                   GLU B
                           56
                                                     72.093
                                                              1.00 25.30
                                            -6.079
                                   34.365
        3459
               CA
                   GLU B
                           56
MOTA
                   GLII R
                           56
                                   35.141
                                            -5.003
                                                     71.334
                                                              1.00 24.31
ATOM
               CB
        3460
                                                     69.836
                                                              1.00 32.15
                                   34.866
                                            -5.039
MOTA
        3461
               CG
                   GLU B
                           56
                                                     69.073
                                                              1.00 31.43
                                   35.512
                                            -3.903
        3462
               CD
                   GLU B
                           56
MOTA
                           56
                                   35.486
                                            -2.759
                                                      69.568
                                                              1.00 28.54
        3463
               OE1
                   GLU B
MOTA
                                                     67.959
                                                              1.00 28.89
                                   36.012
                                            -4.147
MOTA
        3464
               OE2
                   GLU B
                           56
                                                              1.00 28.88
                                                     73.595
        3465
               C
                   GLU B
                           56
                                   34.653
                                            -5.988
MOTA
                                   35.450
                                            -6.766
                                                      74.137
                                                              1.00 25.07
                   GLU B
                          56
ATOM
        3466
               0
                                            ~5.050
                                                      74.272
                                                              1.00 24.52
                                   33.996
        3467
                   LEU B.
                           57
MOTA
               N
                                                     75.702-
                                                              1.00 27.34
        3468
               CA
                   LEU B
                           57
                                   34.203
                                            -4.891
MOTA
                                    33.416
                                            -3.694
                                                      76.231
                                                              1.00 22.79
                           57
                   LEU B
        3469
               CB
ATOM
                                                     75.722
                                            -2.320
                                                              1.00 23.57
                                   33.859
        3470
                   LEU B
                           57
MOTA
               CG
                                                              1.00 22.27
                                                     76.366
        3'471
               CD1 LEU B
                           57
                                    33.008
                                            -1.247
ATOM
                                    35.342
                                             -2.089
                                                      76.061
                                                              1.00 17.24
                   LEU B
                           57
        3472
               CD2
ATOM
                                   33.785
                                             -6.144
                                                              1.00 26.92
                                                      76.452
ATOM
        3473
                   LEU B
                           57
                                                              1.00 24.06
                                                      77.396
                                            -6.568
        3474
                   LEU B
                           57
                                   34.458
               a
MOTA
                                             -6.732
                                                      76.029
                                                              1.00 23.35
        3475
                   LEU B
                           58
                                   32.670
               N
MOTA
                                                      76.674
                                                              1.00 25.60
                                             -7.931
                                   32.154
MOTA
        3476
               CA
                   LEU B
                           58
                                                      76.221
                                                              1.00 28.50
                                            -8.207
        3477
               CB
                   LEU B
                           58
                                    30.718
ATOM
                                                              1.00 30.91
                                    29.734
                                             -7.110
                                                      76.649
                   LEU B
                           58
        3478
               CG
MOTA
                                                      76.212
                                                              1.00 28.93
                                    28.323
                                             -7.468
                           58
ATOM
        3479
               CD1
                   LEU B
                                                              1.00 33.44
                                            -6.945
                                                      78.157
        3480
               CD2
                   LEU B
                           58
                                    29.794
ATOM
                                                              1.00 24.59
                                                      76.446
                                    33.027
                                            -9.153
        3481
                   LEU B
                           58
               C
MOTA
                                                              1.00 19.76
                                   32.760 -10.216
                                                      76.991
                           58
                   LEU B
ATOM
        3482
               a
                                    34.065
                                                      75.630
                                                              1.00 23.99
                                            -9.006
        3483
                   LEU B
                           59
MOTA
               N
                                                              1.00 25.11
                                                      75.411
                   LEU B
                           59
                                    34.988
                                           -10.108
        3484
               CA
ATOM
                                                              1.00 21.64
                                                      74.332
                                    36.018
                                            -9.757
                   LEU B
                           59
        3485
               CB
ATOM
                                                      72.905
                                                              1.00 24.24
                                    35.483
                                             -9.652
        3486
               CG
                   LEU B
                           59
ATOM
                                    36.585
                                                      71.975
                                                              1.00 24.25
                                            -9.177
        3487
               CD1
                   LEU B
                           59
ATOM
                                                      72.468
                                                               1.00 19.91
                                    34.957 -11.014
        3488
               CD2
                   LEU B
MOTA
                                                      76.733
                                                              1.00 23.84
                           59
                                    35.699
                                           -10.371
                   LEU B
        3489
               C
ATOM
                                                               1.00 19.39
                                    36.150
                                                      76.992
                                           -11.489
                           59
        3490
               0
                   LEU B
ATOM
                                                      77.577
                                                               1.00 21.80
                                    35.793
                                             -9.344
        3491
                   PHE B
                           60
               N
ATOM
                                                      78.876
                                                               1.00 23.08
                                             -9.510
                                    36.462
        3492
               CA
                   PHE B
                           60
MOTA
                                                               1.00 18.22
                                                      78.908
                                    37.809
                                             -8.770
               CB
                   PHE B
                           60
        3493
ATOM
                                                               1.00 21.72
                                                      80,230
                                    38.544
                                             -8.906
        3494
               CG
                   PHE B
                           60
ATOM
                                            -10.157
                                                      80.680
                                                               1.00 19.23
                                    38.975
        3495
                   PHE B
                           60
               CD1
ATOM
                                                      81.048
                                                               1.00 17.75
               CD2 PHE B
                           60
                                    38.757
                                             -7.791
        3496
MOTA
                                                               1.00 18.80
                                            -10.301
                                                      81.927
                           60
                                    39.602
                   PHE B
        3497
               CE1
ATOM
                                    39.384
                                             -7.923
                                                      82.297
                                                               1.00 19.23
        3498
               CE2
                   PHE B
                           60
ATOM
                                                      82.737
                                                               1.00 16.10
                                             -9.184
                                    39.807
        3499
               CZ
                   PHE B
                           60
ATOM
                                                      80.083
                                                               1.00 21.58
                                    35.648
                                             -9.069
                   PHE B
                           60
        3500
               C
MOTA
                                                               1.00 22.21
                                    35.508
                                             -9.822
                                                      81.040
LTOM
        3501
               0
                   PHE B
                           60
                                                      80.055
                                                               1.00 20.65
                                             -7.847
                           61
                                    35.128
        3502
              N
                   HIS B
ATOM
                                                               1.00 23.32
                                                      81.184
                   HIS B
                           61
                                    34.362
                                             -7.336
        3503
              CA
MOTA
                                                               1.00 27.60
                                    34.422
                                             -5.807
                                                      81.229
        3504
               CB
                   HIS B
                           61
ATOM
                                             -5.259
                                                      81.440
                                                               1.00 31.83
                                    35.800
                           61
        3505
               CG
                   HIS B
ATOM.
                                                      82.575
                                                               1.00 26.86
              CD2 HIS B
                          61
                                    36.466
                                             -4.940
        3506
ATOM
                                                               1.00 34.35
                                    36.669
                                             -5.003
                                                      80.401
                          61
        3507
              ND1 HIS B
ATOM
                                    37.810
                                             -4.546
                                                      80.887
                                                               1.00 34.78
              CE1 HIS B
                           61
        3508
ATOM
                                                               1.00 36.27
                                                      82.204
                                             -4.499
              NE2 HIS B
                           61
                                    37.713
        3509
ATOM
                                                               1.00 28.04
                                    32.902
                                             -7.775
                                                      81.198
                           61
                   HIS B
        3510
               C
ATOM
                                    32.349
                                                      80.176
                                                               1.00 25.70
                                             -8.167
        3511
               0
                   HIS B
                           61
ATCM
                                                      82.367
                                                               1.00 25.25
                                             -7.691
              N
                   THR B
                           62
                                    32.276
        3512
ATOM
                                                               1.00 25.35
                                                      82.506
                                    30.882
                                             -8.084
                           62
                   THR B
ATOM
        3513
              CA
                                                               1.00 25.47
                                                      83.932
                                    30.578
                                             -8.549
                           62
        3514
               CB
                   THR B
ATOM
                                                               1.00 28.62
                                             -7.462
                                                      84.843
                                    30.783
              0G1
                   THR B
                           62
        3515
ATOM
                                                               1.00 21.32
                                                      84.315
                                    31.482
                                             -9.701
                           62
                  THR B
        3516
              CG2
ATOM
                                                               1.00 26.06
                                             -6.942
                                                      82.162
                                    29.931
                           62
        3517
                   THR B
ATOM
                                             -5.771
                                                               1.00 24.14
                                                      82.254
              0
                   THR B
                           62
                                    30.287
        3518
ATOM
                                                               1.00 28.01
                                                      81.759
                                    28.718
                                             -7.305
                           63
ATCM
                   GLU B
        3519
              N
                                                               1.00 30.77
                                    27.681
                                                      81.389
                           63
                                             -6.349
        3520
              CA
                   GLU B
ATCM
                                                               1.00 33.97
                                                      81.114
                                             -7.094
                           63
                                    26.374
              CB
        3521
```

| ATOM 3522 CG .GLU B 63 | 25.213 -6.210 80.667 3.00.41 13 |
|---|--|
| ATOM 3523 CD GLUB 63 | 25 100 41.12 |
| ATOM 3524 OE1 GLU B 63 | 24 26 21 21 21 21 21 21 21 21 21 21 21 21 21 |
| ATOM 3525 OE2 GLU B 63 | 25 222 |
| ATOM 3526 C GLU B 63 | 22 425 |
| ATOM 3527 O GLU B 63 | 27 301 4 300 02.430 1.00 27.29 |
| ATOM 3528 N ASP B 64 | 22 222 23.13 |
| ATOM 3529 CA ASP B 64 | 27 24.38 |
| ATOM 3530 CB ASP B 64 | 26 207 1.00 29.27 |
| ATOM 3531 CG ASP B 64 | 20 000 100 30.30 |
| ATOM 3532 OD1 ASP B 64 | 20 100 |
| ATOM 3533 OD2 ASP B 64 | 20 210 20 20 20 20 20 20 20 20 20 20 20 20 20 |
| ATOM 3534 C ASP B 64 | 20 200 |
| ATOM 3535 O ASP B 64 | 27 760 -100 20.49 |
| ATOM 3536 N TYR B 65 | 22 222 23.422 1.00 18.33 |
| ATOM 3537 CA TYR B 65 | 20 100 22.75 |
| ATOM 3538 CB TYR B 65 | 3 |
| ATOM 3539 CG TYR B 65 | 20 040 |
| ATOM 3540 CD1 TYR B 65 | 77 007 |
| ATOM 3541 CE1 TYR B 65 | 2.00 21.33 |
| ATOM 3542 CD2 TYR B 65 | 24 20 20 20 40 10 18.32 |
| ATOM 3543 CE2 TYR B 65 | 75 4.5 |
| ATOM 3544 CZ TYR B 65 | 21.00 21.01 |
| ATOM 3545 OH TYR B 65 | 35 35 1.00 20.61 |
| ATOM 3546 C TYR B 65 | 20 200 |
| ATOM 3547 O TYR B 65 | 22 22 22 22 22 22 22 22 22 22 22 22 22 |
| ATOM 3548 N ILE B 66 | 20 10.20 |
| ATOM 3549 CA ILE B 66 | 1.00 13,49 |
| ATOM 3550 CB ILE B 66 | 20 11 19.08 |
| ATOM 3551 CG2 ILE B 66 | 30.208 -2.592 80.432 1.00 23.31 30.200 -1.571 79.303 1.00 21.30 |
| ATOM 3552 CG1 ILE B 66 | 31.400 -3.541 80.260 1.00 27.67 |
| ATOM 3553 CD1 ILE B 66 | 32.758 -2.839 80.291 1.00 29.29 |
| ATOM 3554 C ILE B 66 | 29.128 -0.909 81.940 1.00 26.99 |
| ATOM 3555 O ILE B 66 | 29.294 0.309 81.848 1.00 23 36 |
| ATOM 3556 N ASN B 67 | 27.939 -1.447 82.198 1.00 24.98 |
| ATOM 3557 CA ASN B 67 ATOM 3558 CB ASN B 67 | 26.782 -0.580 82.363 1.00 27.70 |
| 3550 on | 25.492 -1.389 82.580 1 00 25 58 |
| 3560 | 25.081 -2.183 81.341 1.00 26.91 |
| 2561 | 25.199 -1.701 80.220 1.00 31 48 |
| 3001 | 24.572 -3.387 81.545 1.00 23 80 |
| 3563 | 26.982 0.401 83.513 1.00 25 34 |
| 3704 3564 | 40.044 1.539 83 448 1 00 22 52 |
| 3565 63 | 27.064 -0.031 84.568 1.00 23.65 |
| 3566 65 | 27.903 0.863 85.696 1.00 25.25 |
| ATOM 3566 CB THR B 68 ATOM 3567 OG1 THR B 68 | 28.516 0.119 86.891 1.00 29.08 |
| ATOM 3568 CG2 THR B 68 | 27.561 -0.826 87.396 1.00 25.94 |
| ATOM 3569 C THR B 68 | 28.894 1.100 88.002 1.00 22.90 |
| ATOM 3570 O THR B 68 | 28.818 2.009 85.287 1.00 25.91 |
| ATOM 3571 N LEU B 69 | 28.576 3.156 85.661 1.00 28.47 |
| ATOM 3572 CA LEU B 69 | 29.861 1.702 84.519 1.00 25.13 |
| ATOM 3573 CB LEU B 69 | 30.766 2.729 84.054 1.00 24.37 |
| ATOM 3574 CG LEU B 69 | 20 21.32 |
| ATOM 3575 CD1 LEU B 69 | 2.00 22.33 |
| ATOM 3576 CD2 LEU B 69 | 20 22.37 |
| ATOM 3577 C LEU B 69 | 1,00 23,20 |
| ATOM 3578 O LEU B 69 | 23.02 |
| ATOM 3579 N MET B 70 | 20 230 |
| ATOM 3580 CA MET B 70 | 20 440 |
| ATOM 3581 CB MET B 70 | 27 550 21.00 23.87 |
| ATOM 3582 CG MET B 70 | 1.00 24.00 |
| ATOM 3583 SD MET B 70 | |
| ATOM 3584 CE MET B 70 | 1.00 30.35 |
| ATOM 3585 C MET B 70 | 2.500 77.245 1.00 30.20 |
| ATOM 3586 O MET B 70 | 2.002 02.242 1.00 20.02 |
| ATOM 3587 N GLU B 71 | 0.275 00.009 1.00 24.09 |
| | 26.786 4.458 83.194 1.00 28.21 |

| | | | | | | | | 4 00 07 45 |
|-------------|------|-----|--------|----|--------|--------|--------|------------|
| ATOM | 3588 | CA | GLU B | 71 | 25.837 | 5.207 | 84.008 | 1.00 27.45 |
| | | | GLU B | 71 | 25.014 | 4.268 | 84.889 | 1.00 30.70 |
| MOTA | 3589 | CB | | | | | 85.832 | 1.00 33.61 |
| MOTA | 3590 | CG | GLU B | 71 | 24.072 | 5.005 | | |
| | 3591 | CD | GLU B | 71 | 23.044 | 5.867 | 85.096 | 1.00 37.51 |
| MOTA | | | | 71 | 22.333 | 6.638 | 85.773 | 1.00 35.47 |
| MOTA | 3592 | | GLU B | | | | | 1.00 31.03 |
| ATOM | 3593 | OE2 | GLU B | 71 | 22.934 | 5.769 | 83.849 | |
| | 3594 | C | GLU B | 71 | 26.559 | 6.209 | 84.887 | 1.00 29.15 |
| MOTA | | | | | 26.115 | 7.341 | 85.035 | 1.00 23.96 |
| ATOM | 3595 | 0 | GLU B | 71 | | | | 1.00 27.76 |
| ATOM | 3596 | N | ALA B. | 72 | 27.671 | 5.781 | 85.481 | |
| | 3597 | CA | ALA B | 72 | 28.454 | 6.662 | 86.340 | 1.00 27.58 |
| MOTA | | | | | 29.663 | 5.920 | 86.909 | 1.00 23.24 |
| ATOM | 3598 | CB | ALA B | 72 | | | | 1.00 28.07 |
| MOTA | 3599 | С | ALA B | 72 | 28.924 | 7.886 | 85.563 | |
| | | 0 | ALA B | 72 | 28.895 | 8.999 | 86.079 | 1.00 23.22 |
| MOTA | 3600 | | | | 29.356 | 7.684 | 84.322 | 1.00 26.40 |
| MOTA | 3601 | N | GLU B | 73 | | | | 1.00 29.06 |
| MOTA | 3602 | CA | GLU B | 73 | 29.846 | 8.801 | 83.529 | |
| | 3603 | CB | GLU B | 73 | 30.658 | 8.314 | 82.325 | 1.00 29.48 |
| MOTA | | | - | | 31.162 | 9.466 | 81.443 | 1.00 31.00 |
| MOTA | 3604 | CG | GLU B | 73 | | | 80.216 | 1.00 34.37 |
| ATOM | 3605 | CD | GLU B | 73 | 31.938 | 9.009 | | |
| | 3606 | | GLU B | 73 | 33.059 | 8.461 | 80.356 | 1.00 28.41 |
| MOTA | | | | | 31.419 | 9.203 | 79.100 | 1.00 30.59 |
| MOTA | 3607 | OEZ | GLU B | 73 | | | | 1.00 31.92 |
| MOTA | 3608 | С | GLU B | 73 | 28.744 | 9.734 | 83.045 | |
| | 3609 | 0 | GLU B | 73 | 28.894 | 10.951 | 83.104 | 1.00 35.69 |
| MOTA | | | | | 27.633 | 9.186 | 82.570 | 1.00 33.53 |
| ATOM | 3610 | N | ARG B | 74 | | | | 1.00 38.64 |
| ATOM | 3611 | CA | ARG B | 74 | 26.583 | 10.067 | 82.081 | |
| | 3612 | CB | ARG B | 74 | 25.456 | 9.280 | 81.403 | 1.00 39.90 |
| MOTA | | | | 74 | 24.448 | 8.706 | 82.363 | 1.00 46.67 |
| ATOM | 3613 | CG | ARG B | | | | 81.646 | 1.00 47.53 |
| ATOM | 3614 | CD | ARG B | 74 | 23.174 | 8.311 | | |
| | 3615 | NE | ARG B | 74 | 22.076 | 8.153 | 82.594 | 1.00 55.58 |
| MOTA | | | ARG B | 74 | 21.609 | 9.136 | 83.362 | 1.00 56.04 |
| ATOM | 3616 | CZ | | | | 10.351 | 83.297 | 1.00 58.93 |
| MOTA | 3617 | NHl | ARG B | 74 | 22.142 | | | |
| | 3618 | NH2 | ARG B | 74 | 20.601 | 8.910 | 84.192 | 1.00 53.62 |
| MOTA | | | ARG B | 74 | 26.008 | 10.914 | 83.222 | 1.00 35.84 |
| MOTA | 3619 | C | | | 25.778 | 12.107 | 83.048 | 1.00 29.44 |
| MOTA | 3620 | 0 | ARG B | 74 | | | | 1.00 31.02 |
| | 3621 | N | SER B | 75 | 25.794 | 10.302 | 84.386 | |
| MOTA | | CA | SER B | 75 | 25.243 | 11.014 | 85.539 | 1.00 31.99 |
| MOTA | 3622 | | | | 24.592 | 10.038 | 86.510 | 1.00 34.47 |
| MOTA | 3623 | CB | SER B | 75 | | | | 1.00 34.33 |
| MOTA | 3624 | OG | SER B | 75 | 25.581 | 9.228 | 87.123 | |
| | 3625 | C | SER B | 75 | 26.339 | 11.754 | 86.288 | 1.00 35.42 |
| MOTA | | | | 75 | 26.060 | 12.555 | 87.180 | 1.00 33.45 |
| MOTA | 3626 | 0 | SER B | | | | 85.922 | 1.00 33.25 |
| MOTA | 3627 | N | GLN B | 76 | 27.584 | 11.473 | | 1.00 35.61 |
| | 3628 | CA | GLN B | 76 | 28.739 | 12.082 | 86.565 | |
| MOTA | | | GLN B | 76 | 28.818 | 13.572 | 86.241 | 1.00 30.11 |
| MOTA | 3629 | CB | | | | 14.112 | 86.390 | 1.00 39.13 |
| ATOM | 3630 | CG | GLN B | 76 | 30.216 | | 00.320 | 1.00 33.54 |
| | 3631 | CD | GLN B | 76 | 31.124 | 13.681 | 85.248 | |
| ATOM | | OE1 | | 76 | 31.052 | 12.546 | 84.761 | 1.00 29.21 |
| MOTA | 3632 | | | | 31.995 | 14 583 | 84.827 | 1.00 40.93 |
| ATOM | 3633 | NES | | 76 | | | 88.079 | 1.00 37.88 |
| ATOM | 3634 | С | GLN B | 76 | 28.624 | 11 892 | | |
| | 3635 | 0 | GLN B | 76 | 28.901 | 12 308 | 88.858 | 1.00 32.74 |
| MOTA | | | | 77 | 28.209 | 10.697 | 88.488 | 1.00 34.72 |
| MOTA | 3636 | N | SER B | | | | 89.901 | 1.00 37.07 |
| MOTA | 3637 | CA | SER B | 77 | 28.047 | 10.382 | | |
| | 3638 | CB | SER B | 77 | 26.635 | 10.738 | 90.371 | 1.00 39.61 |
| ATOM | | | | 77 | 25.678 | 9.941 | 89.688 | 1.00 39.03 |
| ATOM | 3639 | eg | SER B | | | | 90.112 | 1.00 35.95 |
| ATOM | 3640 | С | SER B | 77 | 28.265 | 8.897 | | 1.00 36.60 |
| | 3641 | 0 | SER B | 77 | 28.177 | 8.108 | 89.173 | |
| ATOM | | | | 78 | 28.528 | 8.518 | 91.355 | 1.00 33.03 |
| MOTA | 3642 | N | VAL B | | | 7.124 | 91.685 | 1.00 33.41 |
| ATOM | 3643 | CA | VAL B | 78 | 28.753 | | | 1.00 36.91 |
| | 3644 | CB | VAL B | 78 | 29.742 | 6.979 | 92.848 | |
| MOTA | | 1 | VAL B | 78 | 29.955 | 5.499 | 93.163 | 1.00 34.37 |
| MOTA | 3645 | | AWD D | | | 7.658 | 92.496 | 1.00 34.19 |
| MOTA | 3646 | CG2 | VAL B | 78 | 31.055 | | | 1.00 34.93 |
| | 3647 | С | VAL B | 78 | 27.461 | 6.431 | 92.082 | |
| MOTA | | õ | VAL B | 78 | 26.897 | 6.703 | 93.143 | 1.00 28.25 |
| ATOM | 3648 | | 222 | | 26.971 | 5.521 | 91.228 | 1.00 36.73 |
| ATOM | 3649 | N | PRO B | 79 | | | | 1.00 37.44 |
| | 3650 | CD | PRO B | 79 | 27.532 | 5.114 | | |
| ATOM | | CA | PRO B | 79 | 25.738 | 4.779 | 91.493 | 1.00 38.33 |
| ATOM | 3651 | | DDO D | | 25.668 | 3.826 | | 1.00 38.68 |
| MOTA | 3652 | CB | PRO B | 79 | | | | 1.00 37.41 |
| ATOM | 3653 | CG | PRO B | 79 | 26.293 | 4.664 | | 2,00 |
| 44 1 1 4171 | | | | | | | _ | |

| ATO | M 3654 | С | PRO | B 79 | | 25.78 | 8 4.0 | 046 92.83 | 34 1 00 36 0 | _ |
|--------------|--------------|----------|----------------|-----------------------|---|------------------|------------------|---------------|--------------------------|----|
| ATO | | | PRO | B 79 | | 26.85 | | | | |
| ATO | | | LYS | | | 24.62 | 3 3.8 | | | |
| ATO | | _ | LYS | | | 24.48 | | | | |
| ATON | | | LYS | | | 23.00 | 3 2.8 | | 7 1.00 43.3 | 3 |
| ATON | | | LYS | | | 22.67 | | | 2 1.00 44.6 | ō |
| ATOM ATOM | | | LYS : | | | 21.19 | _ | | 37 1.00 48.0 | 9 |
| ATOM | | CE NZ | LYS I | | | 20.80 | | | 9 1.00 50.1 | 2 |
| ATOM | | C | LYS I | | | 20.93 | | | | |
| ATOM | | ō | LYS | | | 25.31 | 1 | | | 5 |
| ATOM | | Ň | GLY E | | • | 25.18: 26.17: | | | | |
| ATOM | | CA | GLY E | | | 26.99 | | | | |
| ATOM | | С | GLY E | | | 28.066 | | | | |
| MOTA | | 0 | GLY E | | | 28.861 | | | | 3 |
| MOTA | 3669 | N | ALA E | 82 | | 28.100 | | | | |
| MOTA | | CA | ALA E | | | 29.082 | | | | |
| MOTA | | CB | ALA E | | | 28.755 | | | | |
| MOTA | | С | ALA B | | | 30.517 | | 23 93.40 | | |
| MOTA | 3673 | 0 | ALA B | _ | | 31.461 | | | 5 1.00 32.17 | 'n |
| ATOM | 3674 | N | ARG B | | | 30.677 | | | | ż |
| MOTA | 3675 3676 | CA | ARG B | | - | 31.994 | 2.5 | | 0 1.00 38.75 | 5 |
| MOTA MOTA | 3677 | CB CG | ARG B | 83 | | 31.865 | | | 5 1.00 40.24 | 1 |
| MOTA | 3678 | CD | ARG B | 83 83 | | 33.187 | | | | |
| ATOM | 3679 | NE | ARG B | 83 | | 33.015 34.240 | | | | ò |
| ATOM | 3680 | CZ | ARG B | 83 | | 35.437 | 6.01 5.48 | | |) |
| MOTA | 3681 | NH1 | ARG B | 83 | | 35.598 | 4.17 | | | ĺ |
| ATOM | 3682 | NH2 | ARG B | 83 | | 36.479 | 6.28 | | , | , |
| ATOM - | | | ARG B | 83 | | 32.719 | 1.32 | | | |
| ATOM | 3684 | | ARG B | 83 | | 33.893 | 1.09 | | 1.00 37.18 | |
| MOTA | 3685 | | GLU B | 84 | | 32.011 | 0.56 | 4 96.249 | | |
| ATOM ATOM | 3686 3687 | | GLU B | 84 | | 32.581 | -0.60 | | 1.00 35.29 | |
| ATOM | 3688 | | GLU B GLU B | 84 | | 31.876 | -0.85 | | 1.00 40.14 | |
| ATOM | 3689 | | GLU B | 84 84 | | 30.443 | -0.38 | | | |
| ATOM | 3690 | | GLU B | 84 | | 30.356 29.339 | 1.13 | | | |
| ATOM | | 0E2 (| | 84 | | 31.306 | 1.69 1.76 | | | |
| MOTA | | | SLU B | 84 | | 32.527 | -1.88 | | | |
| MOTA | | | SLU B | 84 | | 33.371 | -2.76 | | | |
| MOTA | | | YS B | 85 | | 31.533 | -1.98 | | | |
| ATOM | | _ | YS B | 85 | | 31.412 | -3.17 | | | |
| ATOM | | | YS B | 85 | | 29.950 | -3.40 | | | |
| ATOM ATOM | | | YS B | 85 | | 29.717 | -4.64 | - | | |
| A OM | | _ | YS B YS B | 85 | | 28.234 | -4.80 | _ | 1.00 32.87 | |
| A.OM | | | YS B | 85 _. 85 | | 28.000 26.582 | -6.04 | | 1.00 34.15 | |
| MGıA | | | YS B | 85 | | 32.267 | -6:18 | | 1.00 35.34 | |
| ATOM | | | YS B | 85 | | 32.817 | -3.096 -4.098 | | 1.00 28.98 | |
| ATOM | 3703 N | | YR B | 86 | | 32.391 | -1.896 | | 1.00 24.69 1.00 27.81 | |
| ATOM | | CA T | YR B | 86 | | 33.141 | -1.692 | | 1.00 27.56 | |
| ATOM | | | YR B | 86 | | 32.206 | -1.050 | | 1.00 28.88 | |
| MOTA | | | YR B | 86 | | 31.008 | -1.927 | 89.951 | 1.00 31.29 | |
| ATOM | | | YR B | 86 | | 31.178 | -3.137 | 89.276 | 1.00 26.99 | |
| MOTA | | | | 86 | | 0.095 | -3.955 | | 1.00 26.97 | |
| MOTA MOTA | | | | 86 | | 9.713 | -1.553 | | 1.00 28.38 | |
| ATOM | | | | 86 86 | | 8.611 | -2.370 | | 1.00 24.19 | |
| ATOM | 3712 0 | | | 86 86 | | 8.815 | ~3.569 | | 1.00 28.46 | |
| ATOM | 3713 C | | | 86 | | 7.747 4.422 | -4.379 | | 1.00 22.70 | |
| ATOM | 3714 0 | | | 86 | | 5.160 | -0.870 -0.645 | | 1.00 24.64 | |
| ATOM | 3715 N | | | 87 | | 4.674 | -0.418 | | 1.00 27.19 1.00 25.54 | |
| MOTA | 3716 C | | | 87 | | 5.881 | 0.341 | | 1.00 29.30 | |
| MOTA | 3717 C | B AS | | 87 | | 7.105 | -0.561 | 92.866 | 1.00 28.92 | |
| ATOM | 3718 C | | | 87 | 3 | 8.343 | 0.019 | 93.506 | 1.00 34.72 | |
| MOTA | 3719 O | D1 AS | ив 8 | 37 | 3 | 8.309 | 0.452 | 94.659 | 1.00 38.41 | |
| | | | | | | | | | | |

| ATOM 3720 NDZ ASN B 87 339.449 0.012 92.775 1.00 35.86 ATOM 3721 C ASN B 87 36.070 1.622 92.223 1.00 29.72 ATOM 3722 O ASN B 87 37.194 1.998 91.876 1.00 24.01 ATOM 3723 N ILE B 88 34.956 2.282 91.932 1.00 29.43 ATOM 3724 CA ILE B 88 34.955 3.536 91.196 1.00 30.64 ATOM 3726 CG ILE B 88 33.891 4.829 89.379 1.00 40.62 ATOM 3726 CG ILE B 88 33.891 4.829 89.379 1.00 40.62 ATOM 3727 CGI ILE B 88 34.421 2.433 89.008 1.00 35.43 ATOM 3728 CDI ILE B 88 34.421 2.433 89.008 1.00 35.43 ATOM 3728 CDI ILE B 88 34.421 2.433 89.008 1.00 35.43 ATOM 3730 O ILE B 88 34.421 2.433 89.008 1.00 31.90 ATOM 3730 O ILE B 88 34.649 1.00 22.686 1.00 29.54 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 31.90 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 31.90 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.421 2.433 89.008 1.00 30.36 ATOM 3731 C ILE B 88 34.451 7.00 32.26 ATOM 3731 C ILE B 89 34.574 7.022 92.686 1.00 29.54 ATOM 3733 C ILE B 89 35.457 8.652 94.177 1.00 37.26 ATOM 3733 C ILE B 89 35.457 8.652 94.177 1.00 37.26 ATOM 3733 C ILE B 89 35.457 8.652 94.177 1.00 37.26 ATOM 3733 C ILE B 89 35.457 8.652 94.177 1.00 37.26 ATOM 3731 C ILE B 89 38.457 8.834 93.103 1.03 30.32 ATOM 3740 C ILE B 90 38.655 7.936 94.247 1.00 31.33 ATOM 3740 C ILE B 90 38.655 7.936 94.247 1.00 31.33 ATOM 3740 C ILE B 90 38.655 7.936 94.247 1.00 31.03 ATOM 3740 C ILE B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3740 C ILE B 91 41.810 9.663 95.405 1.00 22.35 ATOM 3740 C ILE B 91 41.810 9.663 95.405 1.00 22.25 ATOM 3740 C ILE B 91 41.810 9.663 95.405 1.00 22.25 ATOM 3740 C ILE B 91 41.810 9.663 95.405 1.00 22.25 ATOM 3740 C ILE B 91 41.810 9.663 95.405 1.00 22.25 ATOM 3740 C ILE B 91 41.810 9.663 95.405 1.00 22.25 ATOM 3740 C ILE B 91 41.810 9.664 9.30 99.007 1.00 20.47 ATOM 3740 C ILE | | | | | | | | | | | |
|--|------|--------------|-----|--------|----|------|-------|--------|----------------|--------|-------|
| ATOM 3721 C ASN B 87 36.070 1.622 92.223 1.00 29.72 ATOM 3722 O ASN B 87 37.194 1.998 91.876 1.00 24.01 ATOM 3723 N ILE B 88 34.956 2.282 91.932 1.00 29.43 ATOM 3724 CA ILE B 88 34.956 2.282 91.932 1.00 29.43 ATOM 3724 CA ILE B 88 34.956 2.282 91.932 1.00 30.64 ATOM 3725 CB ILE B 88 33.959 3.464 90.027 1.00 37.12 ATOM 3726 CGI ILE B 88 33.959 3.464 90.027 1.00 40.62 ATOM 3727 CGI ILE B 88 33.959 3.464 90.027 1.00 40.62 ATOM 3728 CDI ILE B 88 34.421 2.433 89.008 1.00 15.43 ATOM 3727 C ILE B 88 35.664 2.821 88.324 1.00 41.80 ATOM 3728 CDI ILE B 88 35.664 2.821 89.008 1.00 15.43 ATOM 3737 C ILE B 88 34.483 4.669 92.118 1.00 41.80 ATOM 3731 N GIV B 89 34.574 7.022 92.666 1.00 25.54 ATOM 3731 N GIV B 89 34.574 7.022 92.666 1.00 25.54 ATOM 3733 C GIV B 89 35.601 7.524 93.665 1.00 31.49 ATOM 3734 O GIV B 89 35.5601 7.524 93.665 1.00 31.49 ATOM 3735 N GIV B 90 35.650 7.986 94.177 1.00 37.26 ATOM 3737 N GIV B 90 35.650 7.986 94.999 1.00 30.97 ATOM 3738 O GIV B 90 35.650 7.986 94.999 1.00 30.97 ATOM 3738 O GIV B 90 38.655 7.986 94.999 1.00 31.03 1.00 37.70 ATOM 3737 C GIV B 90 38.655 7.986 94.999 1.00 31.03 1.00 37.70 ATOM 3736 C GIV B 90 38.655 8.344 93.103 1.00 29.39 ATOM 3737 C GIV B 90 38.655 8.344 93.103 1.00 32.78 ATOM 3736 C GIV B 90 38.655 8.344 93.103 1.00 29.39 ATOM 3737 C GIV B 90 38.655 8.344 93.103 1.00 28.15 ATOM 3740 CA TWR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA TWR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA TWR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA TWR B 91 40.820 9.033 95.007 1.00 26.65 ATOM 3740 CA TWR B 91 40.820 9.033 95.007 1.00 26.05 ATOM 3740 CA TWR B 91 40.820 9.033 96.007 1.00 26.05 ATOM 3740 CA TWR B 91 40.820 9.033 96.007 1.00 26.05 ATOM 3740 CA TWR B 91 40.820 9.033 96.007 1.00 28.15 ATOM 3740 CA TWR B 91 40.820 9.033 96.007 1.00 28.15 ATOM 3740 CA TWR B 91 40.820 9.093 97.751 1.00 28.15 ATOM 3740 CA GIV B 92 42.240 6.00 8.330 96.007 1.00 28.55 ATOM 3740 CA GIV B 92 42.240 6.00 8.330 96.007 1.00 28.55 ATOM 3740 CA GIV B 92 42.240 6.00 8.340 97.751 1.00 28.25 ATOM 374 | MOTA | 3720 | ND2 | ASN B | 87 | 3.9 | .449 | 0.012 | 92.775 | | |
| ATOM 3722 O ASN B 87 37.194 1.998 91.876 1.00 24.01 ATOM 3723 N ILE B 88 34.955 2.282 91.932 1.00 29.43 ATOM 3724 CA ILE B 88 34.945 3.556 91.196 1.00 30.64 ATOM 3725 CB ILE B 88 33.995 3.464 90.027 1.00 37.12 ATOM 3726 CG2 ILE B 88 33.995 3.464 90.027 1.00 37.12 ATOM 3727 CG1 ILE B 88 33.921 4.829 89.379 1.00 40.62 ATOM 3727 CG1 ILE B 88 34.421 2.433 89.008 1.00 35.43 ATOM 3737 CC ILE B 88 34.481 2.433 89.008 1.00 35.43 ATOM 3730 O ILE B 88 34.483 4.669 92.118 1.00 31.90 ATOM 3730 O ILE B 88 33.661 4.445 93.024 1.00 24.80 ATOM 3731 N GLY B 89 34.977 5.881 91.875 1.00 30.36 ATOM 3731 N GLY B 89 34.977 5.881 91.875 1.00 30.36 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3736 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3736 C GLY B 90 36.583 6.667 94.005 1.00 30.97 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 31.49 ATOM 3738 N GLY B 90 38.655 7.936 94.247 1.00 31.03 ATOM 3730 N TYR B 91 39.772 8.201 94.915 1.00 32.73 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3742 CG TYR B 91 40.820 9.023 95.359 1.00 28.55 ATOM 3745 CD2 TYR B 91 42.609 9.039 95.359 1.00 28.55 ATOM 3745 CD2 TYR B 91 42.609 9.039 95.359 1.00 28.55 ATOM 3745 CD2 TYR B 91 42.219 7.741 97.208 1.00 28.05 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.586 1.00 28.75 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44.456 6.762 97.594 1.00 28.35 ATOM 3745 CD2 TYR B 91 44. | | | C | ASN B | 87 | 36 | 5.070 | 1.622 | | | |
| ATOM 3723 N ILE B 88 34.956 2.282 91.932 1.00 29.43 ATOM 3724 CA ILE B 88 34.956 2.282 91.932 1.00 29.43 ATOM 3725 CB ILE B 88 33.959 3.464 90.027 1.00 37.12 ATOM 3726 CC2 ILE B 88 33.959 3.464 90.027 1.00 37.12 ATOM 3727 CG1 ILE B 88 33.959 3.464 90.027 1.00 40.62 ATOM 3728 CD1 ILE B 88 34.421 2.433 89.008 1.00 35.43 ATOM 3730 O ILE B 88 34.481 2.2433 89.008 1.00 35.43 ATOM 3731 N GLB 88 34.481 2.2433 89.008 1.00 35.43 ATOM 3731 N GLB 88 34.481 2.2431 89.008 1.00 31.90 ATOM 3731 N GLB 88 34.481 2.2431 89.324 1.00 21.90 ATOM 3731 N GLB 88 34.481 3.681 1.875 1.00 30.36 ATOM 3731 N GLB 89 34.574 7.022 92.6867 1.00 30.36 ATOM 3733 C GLB 89 34.574 7.022 92.6867 1.00 30.36 ATOM 3734 O GLB 89 35.497 8.652 94.177 1.00 37.26 ATOM 3735 N GLB 89 36.585 7.936 94.005 1.00 30.97 ATOM 3736 CA GLB 89 38.455 8.344 93.103 1.00 30.97 ATOM 3737 C GLB 89 93 36.583 7.936 94.247 1.00 30.93 ATOM 3738 O GLB 89 93 38.655 7.936 94.247 1.00 30.93 ATOM 3738 O GLB 89 93 38.655 7.936 94.247 1.00 30.93 ATOM 3738 O GLB 89 93 38.655 7.936 94.247 1.00 30.93 ATOM 3738 O GLB 89 93 38.655 7.936 94.247 1.00 30.93 ATOM 3738 O GLB 89 90 37.612 7.086 94.949 1.00 31.03 ATOM 3738 O GLB 89 91 39.772 8.201 94.915 1.00 32.73 ATOM 3736 C GLB 89 91 39.772 8.201 94.915 1.00 32.73 ATOM 3740 C A TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 C B TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3745 C B TYR B 91 41.810 9.463 95.405 1.00 27.79 ATOM 3745 C B TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3747 C TYR B 91 42.297 6.680 97.751 1.00 27.58 ATOM 3755 C G GLB 92 42.246 6.948 93.318 1.00 28.75 ATOM 3757 C G GLB 92 42.246 6.948 93.318 1.00 28.75 ATOM 3757 C G GLB 92 42.246 6.948 93.318 1.00 28.75 ATOM 3757 C G GLB 92 42.246 6.948 93.318 1.00 28.75 ATOM 3757 C G GLB 92 42.246 6.948 93.318 1.00 28.75 ATOM 3757 C G GLB 92 42.2474 4.726 92.924 1.00 23.35 ATOM 3757 C G GLB 92 42.2474 4.726 92.924 1.00 23.35 ATOM 3758 C GLB 92 42.2474 4.726 92.924 1.00 23.55 ATOM 3766 C ANN B 93 39.534 5.509 89.795 1.00 2.00 2.75 ATOM 3776 C ANN B 93 39.534 5.509 89.795 1.00 2.00 2. | | | | | | 37 | 7.194 | 1.998 | 91.876 | 1.00 2 | 24.01 |
| ATOM 3725 CB ILE B 88 33.945 3.556 91.196 1.00 30.64 ATOM 3725 CG2 ILE B 88 33.959 3.464 90.027 1.00 37.12 ATOM 3727 CG1 ILE B 88 33.821 4.829 89.379 1.00 40.62 ATOM 3727 CG1 ILE B 88 34.421 2.433 89.008 1.00 35.43 ATOM 3729 C ILE B 88 35.684 2.821 88.324 1.00 41.80 ATOM 3730 O ILE B 88 33.681 4.445 97.022 1.00 28.86 ATOM 3731 N GLY B 89 34.577 7.022 97.686 1.00 25.686 ATOM 3731 N GLY B 89 34.577 7.022 97.686 1.00 25.686 ATOM 3732 CA GLY B 89 34.577 7.022 97.686 1.00 25.686 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3733 C GLY B 89 35.407 7.022 97.686 1.00 37.49 ATOM 3734 O GLY B 89 35.407 7.022 97.686 1.00 37.49 ATOM 3735 N GLY B 90 37.612 7.086 94.107 1.00 37.26 ATOM 3737 C GLY B 90 37.612 7.086 94.991 1.00 30.97 ATOM 3738 O GLY B 90 37.612 7.086 94.991 1.00 30.97 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3737 C GLY B 90 38.655 8.344 93.103 1.00 29.39 ATOM 3740 CA 7YR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3740 CA 7YR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA 7YR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3744 CE1 TYR B 91 44.456 6.600 97.751 1.00 28.55 ATOM 3746 CE2 TYR B 91 44.259 7.764 97.208 1.00 28.55 ATOM 3748 OH TYR B 91 44.259 7.764 97.208 1.00 28.55 ATOM 3745 CD GLU B 92 42.247 4.792 97.208 1.00 28.55 ATOM 3755 CD GLU B 92 42.247 4.792 99.294 99.230 90.23 4.322 1.00 28.15 ATOM 3756 CG GLU B 92 42.247 4.792 99.294 99.20 90.20 9 | | | | | | | | 2.282 | 91.932 | 1.00 2 | 29,43 |
| ATOM | | | | | | | | | 91.196 | 1.00 | 30.64 |
| ATOM 3726 CG2 ILLE B 88 33.821 4.829 89,379 1.00 40.62 ATOM 3727 CG1 ILLE B 88 33.421 2.433 89.008 1.00 35.4 ATOM 3728 CD1 ILLE B 88 35.664 2.821 88.324 1.00 41.80 ATOM 3729 C ILLE B 88 34.483 4.669 92.118 1.00 31.90 ATOM 3730 O ILLE B 88 33.681 4.445 93.024 1.00 28.86 ATOM 3731 N GLY B 89 34.977 7.022 92.686 1.00 29.54 ATOM 3731 C GLY B 89 34.977 7.022 92.686 1.00 29.54 ATOM 3732 CA GLY B 89 34.977 7.022 92.686 1.00 29.54 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3734 O GLY B 90 37.612 7.086 94.005 1.00 31.03 ATOM 3735 N GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 37.63 ATOM 3739 N TYR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3737 C GLY B 90 38.655 8.344 93.103 1.00 32.7 ATOM 3739 N TYR B 91 40.820 9.344 93.103 1.00 32.7 ATOM 3734 CG TYR B 91 40.820 9.494 915 1.00 29.39 ATOM 3734 CG TYR B 91 40.820 9.494 915 1.00 29.39 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 29.39 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 28.55 ATOM 3745 CD2 TYR B 91 42.207 6.680 97.094 1.00 31.03 ATOM 3745 CD2 TYR B 91 42.207 6.680 97.094 1.00 32.55 ATOM 3746 CE2 TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CE2 TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3756 CD2 TYR B 91 44.753 5.154 97.637 1.00 27.58 ATOM 3756 CD2 GLU B 92 42.247 4.706 6.80 97.091 1.00 26.59 ATOM 3759 C GLU B 92 42.248 6.124 92.308 1.00 28.55 ATOM 3750 CD GLU B 92 42.248 6.124 92.308 1.00 28.55 ATOM 3750 CD GLU B 92 42.248 6.124 92.308 1.00 28.55 ATOM 3751 CC GLU B 92 42.246 6.124 92.350 1.00 29.30 ATOM 3751 CC GLU B 92 42.246 6.124 92.350 1.00 29.30 ATOM 3751 CC GLU B 92 42.246 6.124 92.350 1.00 29.30 ATOM 3750 CD GLU B 92 42.246 6.124 92.350 1.00 29.30 ATOM 3751 CC GLU B 92 42.246 6.124 92.350 1.00 29.30 ATOM 3756 CD GLU B 92 42.247 4.70 9.70 98.91 1.00 23.42 ATOM 3756 CD GLU B 92 42.246 6.124 92.350 1.00 29.30 ATOM 3757 CC GLU B 92 42.247 4.726 92.924 1.00 23.35 ATOM 3756 CD GLU B 92 42.247 4.72 | | | | | | | | | | 1.00 | 37.12 |
| ATOM 3726 CG1 ILE B 88 33.634 2.433 89.008 1.00 35.43 ATOM 3729 C D1 ILE B 88 35.634 2.821 88.324 1.00 41.80 ATOM 3729 C LLE B 88 35.634 4.665 92.118 1.00 31.90 ATOM 3730 O ILE B 88 33.681 4.485 30.024 1.00 28.86 ATOM 3731 N GLY B 89 34.574 7.022 92.686 1.00 31.90 ATOM 3731 N GLY B 89 34.574 7.022 92.686 1.00 31.90 ATOM 3733 C GLY B 89 35.507 7.022 92.686 1.00 31.90 ATOM 3733 C GLY B 89 35.507 7.022 92.686 1.00 31.90 ATOM 3733 C GLY B 89 35.507 7.022 92.686 1.00 31.90 ATOM 3735 N GLY B 89 35.497 8.652 94.177 1.00 37.26 ATOM 3736 N GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3737 C GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.27 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.27 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 31.03 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 32.73 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.35 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.35 ATOM 3741 CE TYR B 91 42.609 8.330 96.007 1.00 26.05 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.05 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.05 ATOM 3744 CEL TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3746 CEZ TYR B 91 44.403 6.196 97.094 1.00 28.35 ATOM 3747 CZ TYR B 91 44.403 6.196 97.094 1.00 28.35 ATOM 3747 CZ TYR B 91 44.403 6.196 97.094 1.00 28.35 ATOM 3747 CZ TYR B 91 44.404 6.196 97.094 1.00 30.12 ATOM 3747 CZ TYR B 91 44.404 6.196 97.094 1.00 28.35 ATOM 3750 N TYR B 91 44.403 6.196 97.094 1.00 28.35 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.35 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.35 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.35 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.30 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.30 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.30 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.30 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.30 ATOM 3750 N TYR B 91 44.404 6.196 97.094 1.00 28.30 ATOM 3756 N TYR B 91 44.404 6.196 97.094 1.00 28.30 | | | | | | | | | | 1.00 | 40.62 |
| ATOM 3728 CD1 ILE B 88 35.684 2.821 88.324 1.00 41.80 ATOM 3729 C ILE B 88 34.483 4.669 92.118 1.00 31.90 ATOM 3731 N GLY B 88 334.977 5.881 91.875 1.00 30.36 ATOM 3733 C GLY B 89 34.577 7.022 92.686 1.00 28.86 ATOM 3732 CA GLY B 89 34.577 7.022 92.686 1.00 29.54 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3733 N GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3735 N GLY B 90 36.583 6.687 94.005 1.00 30.36 ATOM 3735 N GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3736 CA GLY B 90 38.655 7.936 94.247 1.00 37.28 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 37.98 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 32.73 ATOM 3737 N TYR B 91 39.772 8.201 94.915 1.00 22.39 ATOM 3741 CB TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 27.93 ATOM 3744 CE1 TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3744 CE1 TYR B 91 42.609 8.330 95.359 1.00 28.75 ATOM 3746 CE2 TYR B 91 42.927 6.680 97.751 1.00 27.58 ATOM 3746 CE2 TYR B 91 42.927 6.680 97.751 1.00 27.58 ATOM 3746 CE2 TYR B 91 42.927 6.680 97.751 1.00 27.58 ATOM 3746 CB TYR B 91 44.753 5.154 97.637 1.00 28.23 ATOM 3746 CB TYR B 91 44.753 5.154 97.637 1.00 28.23 ATOM 3746 CB TYR B 91 44.753 5.154 97.637 1.00 28.23 ATOM 3755 CB GLU B 92 42.246 6.164 92.350 1.00 28.32 ATOM 3755 CB GLU B 92 42.246 6.164 92.350 1.00 28.32 ATOM 3755 CB GLU B 92 42.2474 4.726 92.924 1.00 23.35 ATOM 3755 CB GLU B 92 42.246 6.164 92.350 1.00 27.58 ATOM 3755 CB GLU B 92 42.246 6.164 92.350 1.00 27.58 ATOM 3756 CB GLU B 92 42.246 6.164 92.350 1.00 27.59 ATOM 3757 CB GLU B 92 42.246 6.164 92.350 1.00 27.59 ATOM 3757 CB GLU B 92 42.246 6.164 92.350 1.00 27.59 ATOM 3756 CB GLU B 92 42.246 6.164 92.347 1.00 23.35 ATOM 3757 CB GLU B 92 42.246 6.164 92.347 1.00 23.35 ATOM 3756 CB GLU B 92 42.246 6.264 99.962 1.00 23.35 ATOM 3757 CB GLU B 92 42.2474 6.026 6.99 89.962 1.00 23.35 ATOM 3760 CB ANN B 93 39.165 3.329 9.964 1.00 23.161 ATOM 3766 CB ANN B 93 39.165 3.329 9.964 1.00 23.161 ATOM 3767 CB ANN B 93 39.165 | | | | | | | | | | | |
| ATOM 3730 C ILE B 88 34.483 4.669 92.118 1.00 31.90 ATOM 3730 C ILE B 88 33.681 4.445 93.024 1.00 28.67 ATOM 3731 N GLY B 89 34.574 7.022 92.686 1.00 29.57 ATOM 3733 C GLY B 89 34.574 7.022 92.686 1.00 29.57 ATOM 3733 C GLY B 89 35.497 7.022 92.686 1.00 29.57 ATOM 3735 N GLY B 89 35.497 8.652 94.177 1.00 37.26 ATOM 3735 N GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3736 CA GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.37 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.37 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.37 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.37 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.37 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.75 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 27.38 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3742 CG TYR B 91 42.609 8.330 95.359 1.00 28.75 ATOM 3746 CEZ TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3746 CEZ TYR B 91 44.043 6.196 97.094 1.00 30.12 ATOM 3746 CEZ TYR B 91 44.043 6.196 97.094 1.00 28.35 ATOM 3746 CEZ TYR B 91 44.043 6.196 97.094 1.00 28.35 ATOM 3748 OH TYR B 91 44.043 6.196 97.094 1.00 28.35 ATOM 3748 OH TYR B 91 44.043 6.196 97.094 1.00 28.35 ATOM 3748 OH TYR B 91 44.043 6.196 97.094 1.00 28.35 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 28.35 ATOM 3755 CD GLU B 92 42.286 6.124 92.350 1.00 27.58 ATOM 3756 CG GLU B 92 42.286 6.124 92.350 1.00 28.35 ATOM 3756 CD GLU B 92 44.742 1.645 92.294 1.00 23.35 ATOM 3756 CD GLU B 92 44.745 2.298 93.686 1.00 23.35 ATOM 3756 CD GLU B 92 44.745 2.298 93.686 1.00 23.35 ATOM 3760 N ASN B 93 40.314 5.667 90.024 1.00 23.35 ATOM 3760 CD ASN B 93 39.165 4.033 99.887 1.00 23.54 ATOM 3760 CD ASN B 93 39.165 4.033 99.864 1.00 23.90 ATOM 3760 CD ASN B 93 39.165 4.033 99.864 1.00 23.90 ATOM 3760 CD ASN B 93 39.165 4.033 99.864 1.00 23.90 ATOM 3760 CD ASN B 93 39.165 4.033 99.864 1.00 23.90 ATOM 3760 CD ASN B 93 39.165 4.033 99.864 1.00 23.90 ATOM 3760 CD ASN B 93 38.458 6.964 99.997 1.00 23.54 ATOM 3760 CD ASN B 93 38.458 6.366 99.999 | MOTA | | | | | | | | | | |
| ATOM 3730 O ILE B 88 33.681 4.445 93.024 1.00 28.86 ATOM 3731 N GLY B 89 34.977 5.881 91.875 1.00 30.95 ATOM 3732 CA GLY B 89 34.977 7.022 92.686 1.00 29.54 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3734 O GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3735 N GLY B 90 36.583 6.687 94.005 1.00 30.95 ATOM 3736 CA GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 31.73 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3739 N TYR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3739 N TYR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 27.29 ATOM 3743 CDL TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3744 CEL TYR B 91 44.956 6.762 95.896 1.00 27.29 ATOM 3746 CCZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CCZ TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3746 CCZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CCZ TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3746 CCZ TYR B 91 44.456 6.762 97.934 1.00 30.83 ATOM 3748 CDL TYR B 91 44.456 6.762 97.94 1.00 30.93 ATOM 3748 CDL TYR B 91 44.456 6.762 97.94 1.00 30.93 ATOM 3748 CDL TYR B 91 44.456 6.762 97.94 1.00 30.93 ATOM 3748 CDL TYR B 91 44.753 5.154 97.637 1.00 27.58 ATOM 3749 C TYR B 91 44.753 5.154 97.637 1.00 27.58 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 25.22 ATOM 3755 CD GLU B 92 42.286 6.124, 92.350 1.00 29.35 ATOM 3755 CD GLU B 92 42.274 4.726 92.924 1.00 3.35 ATOM 3756 C RAN B 93 39.534 5.509 89.795 1.00 28.75 ATOM 3757 OEZ GLU B 92 42.474 1.645 92.477 1.00 32.53 ATOM 3758 C C GLU B 92 42.274 1.654 92.357 1.00 27.58 ATOM 3757 OEZ GLU B 92 42.274 1.654 92.357 1.00 27.59 ATOM 3757 OEZ GLU B 92 42.276 6.360 97.994 1.00 30.161 ATOM 3757 OEZ GLU B 92 42.276 6.360 97.994 1.00 30.161 ATOM 3757 OEZ GLU B 92 42.276 6.360 97.994 1.00 30.161 ATOM 3758 C C GLU B 92 42.276 6.360 97.994 1.00 30.295 ATOM 3757 OEZ GLU B 92 42.276 6.360 97.995 1.00 22.35 ATOM 3758 C C GLU B 92 42.276 6.360 97.995 1.00 22.35 ATOM 3758 N C C GLU B 9 | MOTA | 3728 | CD1 | | | | | | | | |
| ATOM 3730 O ILE B 88 33.681 4.445 91.022 2.030.36 ATOM 3731 N GLY B 89 34.574 7.022 92.686 1.00 31.96 ATOM 3733 CA GLY B 89 34.574 7.022 92.686 1.00 31.96 ATOM 3734 O GLY B 89 35.497 8.652 94.177 1.00 37.26 ATOM 3735 N GLY B 90 35.497 8.652 94.177 1.00 37.26 ATOM 3736 CA GLY B 90 35.497 8.652 94.177 1.00 37.26 ATOM 3736 CA GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 CC GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.655 8.344 93.103 1.00 32.73 ATOM 3739 N TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA TYR B 91 42.609 8.330 96.007 1.00 26.85 ATOM 3741 CB TYR B 91 42.609 8.330 96.007 1.00 26.85 ATOM 3743 CDI TYR B 91 42.609 8.330 96.007 1.00 26.85 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 44.456 6.762 95.896 1.00 28.55 ATOM 3747 CZ TYR B 91 44.053 6.762 95.896 1.00 28.55 ATOM 3747 CZ TYR B 91 44.053 6.762 95.896 1.00 28.55 ATOM 3747 CZ TYR B 91 44.053 6.762 95.896 1.00 28.55 ATOM 3750 O TYR B 91 44.753 5.154 97.637 1.00 36.59 ATOM 3751 N GLU B 92 42.219 7.741 97.208 1.00 27.58 ATOM 3752 CA GLU B 92 42.286 6.124 92.308 1.00 22.27 ATOM 3751 N GLU B 92 42.286 8.874 92.308 1.00 22.27 ATOM 3755 CD GLU B 92 42.286 8.124 92.311 1.00 29.27 ATOM 3756 CD GLU B 92 42.286 8.124 92.311 1.00 29.80 ATOM 3757 CE GLU B 92 42.286 8.124 92.350 1.00 27.06 ATOM 3756 CD GLU B 92 42.474 1.726 92.324 1.00 23.55 ATOM 3757 CC GLU B 92 42.286 6.124 92.397 1.00 32.15 ATOM 3756 CD GLU B 92 42.474 1.654 92.477 1.00 32.15 ATOM 3757 CC GLU B 92 42.286 6.124 92.927 1.00 23.15 ATOM 3757 CC GLU B 92 42.286 6.324 99.997 1.00 23.2.15 ATOM 3756 CD GLU B 92 42.274 1.645 92.477 1.00 25.26 ATOM 3757 CC GLU B 92 42.274 1.654 92.477 1.00 25.25 ATOM 3756 CD GLU B 92 42.274 1.654 92.477 1.00 25.16 ATOM 3757 CC GLU B 92 42.274 1.00 23.36 89.944 1.00 23.36 ATOM 3758 C GLU B 92 42.274 1.00 23.36 89.941 1.00 24.78 ATOM 3760 CC ASN B 93 37.183 5.839 89.791 1.00 24.78 ATOM 3760 CC ASN B 93 37.183 5. | MOTA | 3729 | С | ILE B | 88 | | | | | | |
| ATOM 3731 N GLY B 89 34.977 5.881 91.873 1.00 329.54 ATOM 3732 CA GLY B 89 34.574 7.022 92.686 1.00 329.54 ATOM 3733 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3735 N GLY B 90 36.583 6.667 94.005 1.00 30.97 ATOM 3735 N GLY B 90 36.583 6.667 94.005 1.00 30.97 ATOM 3736 CA GLY B 90 36.583 6.667 94.005 1.00 30.97 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3739 N TYR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CE TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3750 O TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3750 O TYR B 91 42.219 9.094 9.381 1.00 28.35 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 28.35 ATOM 3755 O GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3755 CD GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3756 OEI GLU B 92 42.286 6.948 93.318 1.00 28.35 ATOM 3757 OEZ GLU B 92 42.286 6.948 93.318 1.00 28.35 ATOM 3757 OEZ GLU B 92 41.568 6.948 93.318 1.00 28.35 ATOM 3757 OEZ GLU B 92 42.286 6.948 93.318 1.00 28.35 ATOM 3757 OEZ GLU B 92 42.286 6.948 93.91 1.00 23.35 ATOM 3757 OEZ GLU B 92 42.2474 1.545 92.977 1.00 32.55 ATOM 3757 OEZ GLU B 92 42.2474 1.545 92.977 1.00 32.55 ATOM 3758 C GLU B 92 42.2474 1.545 92.977 9.90 9.90 9.90 1.00 23.53 ATOM 3757 OEZ GLU B 92 42.2474 9.90 9.997 1.00 23.42 ATOM 3758 OEZ GLU B 92 42.2474 9.90 9.997 1.00 23.55 ATOM 375 | | 3730 | 0 | ILE B | 88 | | | | | | |
| ATOM 3732 CA GIY B 89 34.574 7.022 92.886 1.00 23.35 ATOM 3733 C GIY B 89 35.497 8.652 94.177 1.00 37.26 ATOM 3735 N GIY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3736 CA GIY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GIY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3738 O GIY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3738 O GIY B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3737 CT B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3741 CE TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3743 CDI TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CCZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3747 CZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3748 OH TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3749 C TYR B 91 44.753 5.154 97.637 1.00 36.59 ATOM 3750 O TYR B 91 44.753 5.154 97.637 1.00 30.12 ATOM 3751 N GIU B 92 41.568 6.948 93.318 1.00 22.22 ATOM 3752 CA GIU B 92 42.286 6.124 92.350 1.00 22.33 ATOM 3755 CD GIU B 92 41.568 6.948 93.318 1.00 22.33 ATOM 3756 CB GIU B 92 43.502 3.884 92.221 1.00 28.35 ATOM 3757 OEZ GIU B 92 43.502 3.884 92.221 1.00 28.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 28.35 ATOM 3757 OEZ GIU B 92 43.502 3.884 92.221 1.00 28.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3756 OEI GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GIU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GIU B 92 43.502 3.899 97.10 1.00 32.52 ATOM 3758 C GIU B 92 43.502 3.899 97.10 1.00 32.52 ATOM 3758 C GIU B 92 43.502 3.899 97.10 1.00 23.42 ATOM 3758 C C BASN B 93 39.534 5.509 89.795 1.00 23.42 ATOM 3758 C C BASN B 93 39.534 5.509 89.795 | | 3731 | N | GLY B. | 89 | 34 | 4.977 | | | | |
| ATOM 3734 C GLY B 89 35.601 7.524 93.685 1.00 31.49 ATOM 3734 O GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3735 N GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3736 CA GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3739 N TYR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3743 CDL TYR B 91 42.609 8.330 96.007 1.00 26.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.55 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3747 CZ TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3748 OH TYR B 91 44.043 6.196 97.094 1.00 30.12 ATOM 3749 C TYR B 91 44.043 6.196 97.094 1.00 30.12 ATOM 3750 O TYR B 91 44.553 5.154 97.637 1.00 26.59 ATOM 3750 O TYR B 91 44.566 6.948 93.318 1.00 25.22 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 25.22 ATOM 3755 CO GLU B 92 42.286 6.124 92.350 1.00 25.23 ATOM 3755 OEL GLU B 92 42.286 6.124 92.350 1.00 27.35 ATOM 3756 OEL GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GLU B 92 44.475 2.278 93.687 1.00 23.35 ATOM 3758 C GLU B 92 41.568 6.948 93.318 1.00 28.32 ATOM 3756 OEL GLU B 92 41.568 6.948 99.971 1.00 23.35 ATOM 3757 OEZ GLU B 92 42.286 6.124 92.350 1.00 27.08 ATOM 3758 C GLU B 92 42.742 1.645 92.924 1.00 23.35 ATOM 3757 OEZ GLU B 92 42.286 6.948 99.93 318 1.00 25.22 ATOM 3758 C GLU B 92 42.742 1.645 92.977 1.00 32.155 ATOM 3757 OEZ GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OEZ GLU B 92 43.503 39.534 5.509 89.795 1.00 23.42 ATOM 3757 OEZ GLU B 92 43.503 39.884 92.221 1.00 23.55 ATOM 3760 N ASN B 93 39.534 5.509 89.795 1.00 23.02 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 23.92 ATOM 3760 N ASN B 93 39.534 5.509 89.795 1.00 23.92 ATOM 3761 CA ASN B 93 39.534 6.567 99.024 1.00 23.95 ATOM 3768 C C ASN B 93 | | 3732 | CA | GLY B | 89 | - 34 | 4.574 | | | | |
| ATOM 3735 N GLY B 89 35.497 8.652 94.177 1.00 37.26 ATOM 3735 N GLY B 90 36.683 6.687 94.095 1.00 30.97 ATOM 3736 CA GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3738 O GLY B 91 40.820 9.023 94.322 1.00 22.35 ATOM 3740 CA TYR B 91 40.820 9.023 94.312 1.00 22.15 ATOM 3741 CB TYR B 91 42.609 8.330 96.007 1.00 27.29 ATOM 3743 CDL TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3743 CDL TYR B 91 42.609 8.330 95.405 1.00 27.29 ATOM 3744 CE1 TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CDZ TYR B 91 44.753 5.154 97.637 1.00 30.12 ATOM 3747 CZ TYR B 91 44.753 5.154 97.637 1.00 27.58 ATOM 3749 C TYR B 91 44.753 5.154 97.637 1.00 25.22 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3755 CD GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3755 CD GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3755 CD GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3756 O CEI GLU B 92 42.474 4.752 92.924 1.00 23.35 ATOM 3756 CD GLU B 92 42.474 1.594 6.024 90.997 1.00 23.42 ATOM 3756 CD GLU B 92 42.474 1.594 6.024 90.997 1.00 23.42 ATOM 3756 CD GLU B 92 42.474 1.594 6.024 90.997 1.00 23.42 ATOM 3756 CD GLU B 92 42.474 1.594 6.024 90.997 1.00 23.42 ATOM 3760 N ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3761 CA ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3761 CA ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3760 CA ASN B 93 39.305 10.393 89.664 1.00 23.90 ATOM 3761 CA ASN B 93 39.305 10.393 89.664 1.00 23.75 ATOM 3760 CA ASN B 93 39.305 10.393 89.716 1.00 12.55 ATOM 3776 CA ASN B 93 39.305 10.393 89.716 1.00 25.50 | | | С | GLY B | 89 | 3 5 | 5.601 | | | | |
| ATOM 3735 N GLY B 90 36.583 6.687 94.005 1.00 30.97 ATOM 3736 CA GLY B 90 37.612 7.086 94.949 1.00 31.03 ATOM 3737 C GLY B 90 38.455 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3739 N TYR B 91 39.772 8.201 94.915 1.00 29.39 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.55 ATOM 3743 CD1 TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3744 CEI TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3745 CD2 TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3746 CE2 TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3747 CZ TYR B 91 44.043 6.196 97.094 1.00 30.12 ATOM 3748 OH TYR B 91 44.043 6.196 97.094 1.00 30.12 ATOM 3749 C TYR B 91 44.553 8.271 93.226 1.00 29.27 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3751 N GLU B 92 41.563 8.271 93.226 1.00 29.27 ATOM 3752 CA GLU B 92 41.566 6.948 93.318 1.00 22.335 ATOM 3755 CD GLU B 92 42.286 6.124 92.350 1.00 28.35 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 22.335 ATOM 3756 OEI GLU B 92 43.502 3.884 92.221 1.00 22.335 ATOM 3757 OEZ GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3758 C GLU B 92 43.502 3.884 92.221 1.00 22.342 ATOM 3759 O GLU B 92 42.246 6.260 89.962 1.00 33.54 ATOM 3756 OEI GLU B 92 43.502 3.884 92.221 1.00 22.355 ATOM 3757 OEZ GLU B 92 42.246 6.260 89.962 1.00 33.54 ATOM 3758 C GLU B 92 42.246 6.260 89.962 1.00 33.64 ATOM 3759 O GLU B 92 42.242 6.260 89.962 1.00 32.42 ATOM 3760 C ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3760 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3761 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3760 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3761 C ASN B 93 39.368 6.362 89.944 1.00 23.42 ATOM 3763 C G ASN B 93 39.165 6.362 89.944 1.00 23.42 ATOM 3760 C ASN B 93 39.266 6.362 89.944 1.00 23.42 ATOM 3761 C ASN B 93 39.266 6.362 89.944 1.00 23.42 ATOM 3762 C B ASN B 93 39.266 6.362 89.944 1.00 23.95 ATOM 3760 C ASN B 93 39.266 6.363 89.710 1.00 22.55 ATOM 3777 C B VAL B 95 32.606 89.962 | | | | GLY B | 89 | 35 | 5.497 | 8.652 | 94.177 | | |
| ATOM 3736 CA GLY B 90 37.612 7.086 94.949 1.00 31.78 ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.78 ATOM 3738 O GLY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3738 O TYR B 91 39.772 8.201 94.915 1.00 28.35 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 26.60 ATOM 3743 CD1 TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3744 CC TYR B 91 44.456 6.762 95.896 1.00 28.75 ATOM 3745 CD2 TYR B 91 42.927 6.680 97.751 1.00 27.58 ATOM 3746 CE2 TYR B 91 42.927 6.680 97.751 1.00 27.58 ATOM 3747 CZ TYR B 91 42.927 6.680 97.751 1.00 27.58 ATOM 3748 OH TYR B 91 44.753 5.154 97.637 1.00 30.12 ATOM 3749 C TYR B 91 44.753 5.154 97.637 1.00 30.12 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 28.32 ATOM 3751 N GLU B 92 41.563 8.271 93.226 1.00 29.27 ATOM 3752 CB GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3755 CD GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3755 CD GLU B 92 42.474 4.726 92.924 1.00 23.80 ATOM 3756 OE1 GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3757 OE2 GLU B 92 42.474 4.726 92.924 1.00 23.80 ATOM 3756 CB GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3757 OE2 GLU B 92 42.474 1.645 92.477 1.00 31.61 ATOM 3761 CA SAN B 93 40.314 5.677 91.007 1.00 24.78 ATOM 3762 CB SAN B 93 40.314 5.677 91.007 1.00 24.78 ATOM 3761 CA SAN B 93 40.314 5.677 91.007 1.00 24.78 ATOM 3763 CB ASN B 93 40.314 5.677 91.007 1.00 22.35 ATOM 3761 CA SAN B 93 40.314 5.677 91.007 1.00 22.35 ATOM 3761 CA SAN B 93 40.314 5.677 91.007 1.00 22.35 ATOM 3763 CB GLU B 92 41.594 6.024 90.997 1.00 23.45 ATOM 3766 CB ASN B 93 40.314 5.677 91.007 1.00 22.55 ATOM 3767 O ASN B 93 40.314 5.677 91.007 1.00 22.35 ATOM 3766 CB ASN B 93 40.314 5.677 91.007 1.00 22.55 ATOM 3767 O ASN B 93 40.314 5.677 91.007 1.00 22.55 ATOM 3766 CB ASN B 93 40.314 5.677 91.007 1.00 22.55 ATOM 3767 O ASN B 93 40.314 5.677 91.007 1.00 22.55 ATOM 3767 O ASN B 93 40.314 5.677 91.007 1.00 22.55 ATOM 3768 CB ASN B 93 40.324 8.499 7.693 88.791 1.00 22.55 ATOM 3767 O ASN B 93 40.324 8.499 7.693 88.791 1.00 22.55 ATOM 3776 CB ASN B 93 40. | | - | | | | 3 (| 6.583 | 6.687 | 94.005 | | |
| ATOM 3737 C GLY B 90 38.655 7.936 94.247 1.00 34.73 ATOM 3738 O GLY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3739 N TYR B 91 40.820 9.023 94.312 1.00 29.39 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.00 28.75 ATOM 3741 CB TYR B 91 42.609 8.330 96.007 1.00 26.65 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 26.55 ATOM 3743 CD1 TYR B 91 42.609 8.330 96.007 1.00 28.75 ATOM 3744 CEI TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3745 CD2 TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CD2 TYR B 91 42.219 7.741 97.208 1.00 28.75 ATOM 3746 CD2 TYR B 91 44.043 6.196 97.094 1.00 30.15 ATOM 3746 CD2 TYR B 91 44.043 6.196 97.094 1.00 30.55 ATOM 3746 CD2 TYR B 91 44.043 6.196 97.094 1.00 30.55 ATOM 3745 C TYR B 91 44.043 6.196 97.094 1.00 30.55 ATOM 3745 C TYR B 91 44.153 5.154 97.637 1.00 26.55 ATOM 3750 C TYR B 91 42.109 8.874 92.308 1.00 25.27 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 28.32 ATOM 3755 CD GLU B 92 42.246 6.124 92.350 1.00 27.36 ATOM 3755 CD GLU B 92 42.246 6.124 92.235 1.00 23.35 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 44.475 92.247 1.00 32.15 ATOM 3756 CD GLU B 92 44.475 92.248 1.00 33.65 ATOM 3755 CD GLU B 92 44.575 2.278 93.678 1.00 31.61 ATOM 3756 CD GLU B 92 44.475 92.947 1.00 32.15 ATOM 3756 CD GLU B 92 44.475 92.947 1.00 32.15 ATOM 3756 CD GLU B 92 44.500 3.884 92.221 1.00 29.80 ATOM 3756 CD GLU B 92 44.500 3.884 92.221 1.00 29.80 ATOM 3756 CD GLU B 92 44.500 3.884 92.221 1.00 29.80 ATOM 3757 CD GLU B 92 44.475 92.947 92.94 1.00 32.42 ATOM 3757 CD GLU B 92 44.500 3.884 92.221 1.00 23.61 ATOM 3757 CD GLU B 92 44.500 3.884 92.221 1.00 23.55 ATOM 3760 CD ASN B 93 39.165 40.03 38.646 1.00 23.90 ATOM 3761 CA ASN B 93 39.165 40.03 38.646 1.00 23.90 ATOM 3761 CA ASN B 93 39.165 40.03 38.678 1.00 24.78 ATOM 3761 CA ASN B 93 39.165 40.03 38.846 99.942 1.00 25.16 ATOM 3760 CD ASN B 93 39.366 8.300 99.941 1.00 24.78 ATOM 3760 CD ASN B 93 39.366 8.300 99.941 1.00 24 | | | | | | 3. | 7.612 | 7.086 | 94.949 | 1.00 | 31.03 |
| ATOM 3738 O GLY B 90 38.455 8.344 93.103 1.00 32.73 ATOM 3739 N TYR B 91 40.820 9.023 94.322 1.00 28.15 ATOM 3740 CA TYR B 91 41.810 9.463 95.405 1.00 26.60 ATOM 3740 CG TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3743 CDI TYR B 91 42.609 8.330 96.007 1.00 26.60 ATOM 3743 CDI TYR B 91 44.456 6.762 95.896 1.00 28.55 ATOM 3744 CE1 TYR B 91 44.456 6.762 95.896 1.00 28.55 ATOM 3745 CDZ TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3745 CDZ TYR B 91 42.227 6.680 97.751 1.00 27.36 ATOM 3746 CE2 TYR B 91 42.227 6.680 97.751 1.00 27.36 ATOM 3748 OH TYR B 91 44.753 5.154 97.637 1.00 30.12 ATOM 3748 OH TYR B 91 44.753 5.154 97.637 1.00 30.12 ATOM 3750 O TYR B 91 42.509 8.874 92.308 1.00 25.22 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 25.22 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3756 OE GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3756 OE GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3757 OE2 GLU B 92 44.755 2.500 92.827 1.00 30.61 ATOM 3758 C GLU B 92 44.755 2.500 92.826 1.00 35.34 ATOM 3756 OE GLU B 92 44.755 2.78 93.678 1.00 31.61 ATOM 3756 C GLU B 92 42.204 6.024 90.997 1.00 23.42 ATOM 3756 OE GLU B 92 42.204 6.024 90.997 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.024 90.997 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3757 OE2 GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GRU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GRU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 C GRU B 92 43.500 89.887 1.00 23.42 ATOM 3761 C G ASN B 93 39.534 5.509 89.795 1.00 23.42 ATOM 3761 C G ASN B 93 39.534 5.509 89.795 1.00 23.42 ATOM 3761 C G ASN B 93 39.534 5.509 89.795 1.00 23.90 ATOM 3761 C G ASN B 93 39.534 5.509 89.887 1 | | | | | | | | 7.936 | 94.247 | 1.00 | 34.78 |
| ATOM 3739 N TYR B 91 40.820 9.023 94.322 1.000 29.39 ATOM 3740 CA TYR B 91 40.820 9.023 94.322 1.000 28.15 ATOM 3741 CB TYR B 91 41.810 9.463 95.405 1.00 27.29 ATOM 3742 CG TYR B 91 42.609 8.330 96.007 1.00 28.65 ATOM 3744 CEI TYR B 91 42.609 8.330 96.007 1.00 28.55 ATOM 3745 CD2 TYR B 91 42.456 6.762 95.896 1.00 28.75 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3746 CEZ TYR B 91 42.219 7.741 97.208 1.00 28.35 ATOM 3746 CEZ TYR B 91 44.043 6.196 97.0751 1.00 27.58 ATOM 3746 CEZ TYR B 91 44.043 6.196 97.094 1.00 30.15 ATOM 3747 CZ TYR B 91 44.043 6.196 97.094 1.00 30.15 ATOM 3748 OH TYR B 91 44.153 8.271 93.226 1.00 27.58 ATOM 3750 O TYR B 91 42.503 8.271 93.226 1.00 28.32 ATOM 3751 N GLU B 92 42.286 6.124 92.308 1.00 25.22 ATOM 3752 CA GLU B 92 42.286 6.124 92.305 1.00 27.35 ATOM 3755 CD GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3756 OEI GLU B 92 43.502 3.884 92.221 1.00 23.35 ATOM 3756 OEI GLU B 92 44.475 2.278 93.677 1.00 32.15 ATOM 3757 OEZ GLU B 92 44.475 2.278 93.677 1.00 32.15 ATOM 3758 C GLU B 92 44.475 2.278 93.678 1.00 21.96 ATOM 3756 OEI GLU B 92 44.475 2.278 93.678 1.00 21.96 ATOM 3756 OEI GLU B 92 42.204 6.6260 89.962 1.00 20.47 ATOM 3756 OEI GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 OEI GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 OEI GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 OEI GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 OEI GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3756 OEI GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3757 OE GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3758 C GLU B 92 42.204 6.260 89.962 1.00 23.42 ATOM 3760 N ASN B 93 39.165 4.033 89.664 1.00 23.96 ATOM 3761 CA SN B 93 39.165 4.033 89.664 1.00 23.96 ATOM 3762 C B ASN B 93 39.165 4.033 89.946 1.00 23.95 ATOM 3766 C RASN B 93 39.165 4.038 89.941 1.00 24.78 ATOM 3767 O RASN B 93 39.165 4.038 89.941 1.00 24.78 ATOM 3767 O RASN B 93 39.165 4.038 89.941 1.00 22.55 ATOM 3768 N PRO B 94 36.362 89.942 1.00 22.55 ATOM 3776 C C PRO B 94 36.362 89.942 1.00 23.95 ATOM 3777 C C PRO B 94 36.362 | | | | | | | | | 93.103 | 1.00 | 32.73 |
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| ATOM 3746 C2 TYR B 91 44.043 6.196 97.094 1.00 30.12 ATOM 3748 OH TYR B 91 44.753 5.154 97.637 1.00 36.59 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3751 N GLU B 92 41.563 6.948 93.318 1.00 28.52 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3756 OEI GLU B 92 44.474 2.269 92.924 1.00 23.35 ATOM 3756 OEI GLU B 92 42.742 1.645 92.477 1.00 35.34 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 44.204 6.260 89.962 1.00 20.47 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3764 CG ASN B 93 40.351 3.120 89.943 1.00 24.36 ATOM 3766 C ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 C ASN B 93 39.165 4.033 89.867 1.00 22.35 ATOM 3766 C ASN B 93 39.165 4.033 89.867 1.00 22.35 ATOM 3766 C ASN B 93 39.165 4.033 89.867 1.00 22.35 ATOM 3766 C ASN B 93 39.165 4.033 89.887 1.00 22.35 ATOM 3767 O ASN B 93 39.183 5.849 9.944 1.00 25.16 ATOM 3767 O ASN B 93 39.738 8.389 89.716 1.00 13.35 ATOM 3767 O ASN B 93 39.738 8.389 89.716 1.00 20.91 ATOM 3767 O ASN B 93 39.738 8.389 89.716 1.00 22.35 ATOM 3767 O ASN B 93 39.738 8.389 89.716 1.00 22.35 ATOM 3767 O ASN B 93 39.738 8.389 89.716 1.00 22.35 ATOM 3769 CD PRO B 94 38.247 9.972 90.200 1.00 25.95 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 33.317 9.812 88.103 1.00 22.67 ATOM 3776 CA PRO B 94 36.366 81.77 88.873 1.00 22.69 ATOM 3778 CGI VAL B 95 33.375 9.346 89.622 1.00 27.59 ATOM 3778 CGI VAL B 95 33.375 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 33.375 9.346 89.622 1.00 27.59 ATOM 3781 C VAL B 95 33.375 9.346 89.622 1.00 27. | ATOM | 3745 | CD2 | | | | | | | | |
| ATOM 3747 CZ TYR B 91 44.043 5.196 97.037 1.00 36.59 ATOM 3748 OH TYR B 91 44.753 5.154 97.637 1.00 36.59 ATOM 3750 O TYR B 91 41.563 8.271 93.226 1.00 29.27 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3751 N GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 29.80 ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 35.34 ATOM 3755 CD GLU B 92 44.475 2.278 93.678 1.00 32.15 ATOM 3755 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3755 OE2 GLU B 92 44.475 2.278 93.678 1.00 23.42 ATOM 3759 O GLU B 92 41.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3761 CA ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3762 CB ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 OD1 ASN B 93 40.311 5.677 91.017 1.00 18.85 ATOM 3766 OD1 ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 OD ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3767 NOZ ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3768 N PRO B 94 38.249 7.693 89.887 1.00 13.35 ATOM 3766 C ASN B 93 39.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 C PRO B 94 38.449 7.693 89.887 1.00 25.16 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3775 C PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3778 CG VAL B 95 33.035 10.885 87.664 1.00 25.94 ATOM 3778 CG VAL B 95 33.035 10.885 87.664 1.00 25.94 ATOM 3781 O VAL B 95 33.035 10.885 87.664 1.00 25.94 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 25.99 ATOM 3784 CB SER B 96 35.199 11.647 84.868 1.00 24.82 | MOTA | 3746 | CE2 | TYR B | | | | | | | |
| ATOM 3748 OH TYR B 91 44.753 8.271 93.226 1.00 29.27 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3751 N GLU B 92 41.563 6.948 93.318 1.00 28.232 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.505 2.500 92.826 1.00 35.34 ATOM 3756 OEI GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 21.61 ATOM 3759 O GLU B 92 44.475 2.278 93.678 1.00 21.61 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 .00 18.85 ATOM 3761 CA ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3762 CB ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 C ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 ND2 ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 39.738 8.389 89.716 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 39.738 8.889.716 1.00 20.91 ATOM 3767 O ASN B 93 38.285 6.366 89.942 1.00 25.56 ATOM 3767 O ASN B 93 38.285 6.366 89.942 1.00 25.56 ATOM 3767 O ASN B 93 39.738 8.8887 1.00 26.37 ATOM 3767 O ASN B 93 38.285 6.366 89.942 1.00 25.77 ATOM 3768 C C PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3770 CA PRO B 94 36.566 81.76 87.808 1.00 25.95 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3773 C PRO B 94 36.366 81.77 88.873 1.00 22.607 ATOM 3775 N VAL B 95 33.035 10.393 88.742 1.00 23.75 ATOM 3778 CGI VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3778 CGI VAL B 95 33.375 9.346 89.622 1.00 27.59 ATOM 3778 CGI VAL B 95 35.564 11.793 87.6641 1.00 25.95 ATOM 3781 O VAL B 95 35.564 11.793 87.6641 1.00 2 | | 3747 | CZ | TYR B | 91 | | | | | | |
| ATOM 3749 C TYR B 91 41.563 8.271 93.226 1.00 25.22 ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 25.22 ATOM 3751 N GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.474 4.726 92.924 1.000 23.35 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 35.34 ATOM 3755 OE2 GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3758 C GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3759 O GLU B 92 41.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 41.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3758 C GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.534 5.509 89.795 1.00 22.35 ATOM 3764 OD1 ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3764 OD1 ASN B 93 40.315 3.120 89.943 1.00 24.78 ATOM 3766 C ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3766 ND2 ASN B 93 40.240 2.311 90.987 1.00 22.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 22.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 36.562 81.76 87.808 1.00 22.50 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 25.95 ATOM 3773 C PRO B 94 36.562 81.76 87.808 1.00 25.95 ATOM 3773 C PRO B 94 36.562 81.76 87.808 1.00 25.95 ATOM 3773 C PRO B 94 36.562 81.76 87.808 1.00 25.95 ATOM 3779 CG2 VAL B 95 34.317 9.812 88.103 1.00 25.95 ATOM 3779 CG2 VAL B 95 34.317 9.812 88.103 1.00 25.95 ATOM 3780 C VAL B 95 34.317 9.812 88.103 1.00 25.9 | | 3748 | OH | TYR B | 91 | | | | | 1.00 | 20.22 |
| ATOM 3750 O TYR B 91 42.109 8.874 92.308 1.00 28.32 ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 28.32 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3754 CG GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 35.34 ATOM 3756 OEI GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3750 OE GLU B 92 42.204 6.024 90.997 1.00 23.42 ATOM 3750 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.962 1.00 20.47 ATOM 3763 CG ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 ODI ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 40.351 3.120 89.944 1.00 23.35 ATOM 3766 C ASN B 93 40.351 3.120 89.944 1.00 25.16 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 29.91 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3768 O C VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3770 CA PRO B 94 36.562 8.176 89.887 1.00 25.77 ATOM 3771 CB PRO B 94 36.562 8.176 89.887 1.00 25.77 ATOM 3772 CG PRO B 94 36.562 8.176 89.887 1.00 25.75 ATOM 3773 CB VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3774 O PRO B 94 36.562 8.176 89.622 1.00 27.59 ATOM 3778 CG1 VAL B 95 34.317 9.812 88.103 1.00 25.95 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 25 | | 3749 | С | TYR B | 91 | 4 | 1.563 | | | | |
| ATOM 3751 N GLU B 92 41.568 6.948 93.318 1.00 27.06 ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3754 CG GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3756 OE1 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 44.475 2.278 93.678 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.554 5.509 89.962 1.00 20.47 ATOM 3760 C ASN B 93 39.554 5.509 89.962 1.00 21.96 ATOM 3763 CG ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3764 OD1 ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 C ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 23.50 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3760 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3760 C ASN B 93 38.285 6.362 89.944 1.00 26.37 ATOM 3760 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3760 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3760 C ASN B 93 38.285 6.362 89.944 1.00 26.37 ATOM 3760 C ASN B 93 38.285 6.362 89.944 1.00 26.37 ATOM 3760 C A RO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3760 C A RO B 94 39.297 9.740 89.223 1.00 22.50 ATOM 3770 C A RO B 94 39.297 9.740 89.223 1.00 22.50 ATOM 3771 C B PRO B 94 36.562 8.176 89.223 1.00 25.95 ATOM 3773 C PRO B 94 36.562 8.176 89.223 1.00 25.95 ATOM 3773 C PRO B 94 36.562 8.176 89.223 1.00 25.95 ATOM 3775 C PRO B 94 36.562 8.176 89.223 1.00 25.95 ATOM 3775 C PRO B 94 36.562 8.176 89.223 1.00 25.95 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 27.14 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.067 10.861 87.175 1.00 25.69 ATOM 3781 C VAL B 95 32.067 10.861 87.175 1.00 25.96 ATOM 3780 C VAL B 95 32.067 10.861 87.175 1.00 25.90 ATOM 3781 C VAL B 95 32.067 10.861 87.175 1.00 | | | 0 | TYR B | 91 | | | | | | |
| ATOM 3752 CA GLU B 92 42.286 6.124 92.350 1.00 27.06 ATOM 3753 CB GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 35.34 ATOM 3756 OE1 GLU B 92 44.772 2.278 93.678 1.00 31.61 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3759 O GLU B 92 44.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3765 ND2 ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3766 C ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 40.240 2.311 90.987 1.00 25.16 ATOM 3767 O ASN B 93 40.240 2.311 90.987 1.00 25.16 ATOM 3767 CA PRO B 94 38.449 7.693 89.887 1.00 25.16 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 24.59 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3775 CA VAL B 95 34.317 9.812 88.103 1.00 25.97 ATOM 3775 CA VAL B 95 32.376 9.346 89.622 1.00 27.14 ATOM 3775 CA VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 25.95 ATOM 3781 CG VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 25.95 ATOM 3781 CG VAL B 95 32.376 9.346 89.622 1.0 | | | N | GLU B | 92 | 4 | 1.568 | | | _ | |
| ATOM 3753 CB GLU B 92 42.474 4.726 92.924 1.00 23.35 ATOM 3754 CG GLU B 92 43.502 3.884 92.221 1.00 29.80 ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 35.34 ATOM 3756 OEI GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 44.475 2.278 93.678 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.534 5.509 89.795 1.00 22.379 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 ODI ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.997 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3773 C PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 25.77 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.95 ATOM 3777 CB VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 35.564 11.793 87.661 1.00 25.625 ATOM 3781 O VAL B 95 35.564 11.793 87.661 1.00 25.25 ATOM 3782 N SER B 96 34.912 10.861 87.175 1.00 25.05 ATOM 3784 CB SER B 96 36.729 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.647 84.868 1.00 24.82 | | | | GLU B | 92 | 4 | 2.286 | 6.124. | | | |
| ATOM 3754 CG GLU B 92 43.502 3.884 92.221 1.00 25.84 ATOM 3755 CD GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3757 OE2 GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3758 C GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3761 CA ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 C ASN B 93 41.362 3.160 89.239 1.00 22.35 ATOM 3766 C ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3769 CD PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3770 CA PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3770 CA PRO B 94 38.449 7.693 89.887 1.00 24.59 ATOM 3770 CA PRO B 94 38.449 7.693 89.887 1.00 25.95 ATOM 3770 CA PRO B 94 38.449 7.693 89.887 1.00 25.95 ATOM 3770 CA PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3770 CA PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 25.77 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 25.77 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 27.14 ATOM 3777 CB VAL B 95 32.376 9.346 89.622 1.00 27.14 ATOM 3777 CB VAL B 95 32.376 9.346 89.622 1.00 27.14 ATOM 3777 CB VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 25.95 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 25.95 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 25.95 ATOM 3781 CA SER B 96 34.708 10.647 84 | | | | | 92 | 4 | 2.474 | 4.726 | | | |
| ATOM 3755 CD GLU B 92 43.585 2.500 92.826 1.00 35.34 ATOM 3756 OE1 GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 44.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3763 CG ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 ND2 ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 13.35 ATOM 3769 CD PRO B 94 39.7378 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.7378 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.5.95 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 27.59 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3783 CA SER B 96 34.708 10.647 84.868 1.00 24.82 ATOM 3781 O VAL B 95 35.564 11.793 87.661 1.00 25.95 ATOM 3781 CA SER B 96 34.708 10.647 84.868 1.00 24.82 ATOM 3783 CA SER B 96 34.708 10.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 34.708 10.647 84.860 1.00 25.95 | | | | | 92 | 4 | 3.502 | 3.884 | | | |
| ATOM 3756 OE1 GLU B 92 42.742 1.645 92.477 1.00 32.15 ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 41.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.165 4.033 89.943 1.00 24.78 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 OD1 ASN B 93 40.351 3.120 89.943 1.00 22.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3767 OA ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 25.16 ATOM 3770 CA PRO B 94 39.297 9.740 89.223 1.00 25.90 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 25.77 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 22.60 ATOM 3775 N VAL B 95 34.317 9.812 88.103 1.00 25.77 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.77 ATOM 3776 CA VAL B 95 32.067 10.855 87.662 1.00 27.14 ATOM 3778 CG VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 35.564 11.793 87.661 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.661 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.661 1.00 25.90 ATOM 3783 CA SER B 96 34.708 10.669 85.871 1.00 25.90 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10 | | | | | | 4 | 3.585 | 2.500 | 92.826 | | |
| ATOM 3757 OE2 GLU B 92 44.475 2.278 93.678 1.00 31.61 ATOM 3758 C GLU B 92 41.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.26 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 OD1 ASN B 93 41.362 3.160 89.239 1.00 22.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3776 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 25.95 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3774 O PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 25.95 ATOM 3776 CA VAL B 95 32.367 10.855 87.662 1.00 25.69 ATOM 3777 CB VAL B 95 32.367 10.855 87.662 1.00 25.69 ATOM 3778 CG1 VAL B 95 32.367 10.855 87.662 1.00 25.69 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3782 N SER B 96 34.708 10.669 85.871 1.00 28.02 ATOM 3781 O VAL B 95 35.564 11.793 87.6641 1.00 25.69 ATOM 3783 CA SER B 96 34.708 10.669 85.871 1.00 25.90 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.90 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 34.708 10.669 85.871 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.647 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 | | | | | | 4 | 2.742 | 1.645 | 92 .477 | | |
| ATOM 3758 C GLU B 92 41.594 6.024 90.997 1.00 23.42 ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3764 OD1 ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.562 81.76 87.808 1.00 25.77 ATOM 3774 O PRO B 94 36.562 81.76 87.808 1.00 25.77 ATOM 3775 C PRO B 94 36.562 81.76 87.808 1.00 25.77 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 25.94 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 27.14 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 26.34 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 35.564 11.793 87.641 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.95 ATOM 3782 N SER B 96 34.708 10.669 85.871 1.00 25.95 ATOM 3782 N SER B 96 34.708 10.669 85.871 1.00 25.90 ATOM 3782 N SER B 96 34.708 10.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.647 84.865 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.647 84.865 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.72 | | | | | | 4 | 4.475 | 2.278 | 93.678 | | |
| ATOM 3759 O GLU B 92 42.204 6.260 89.962 1.00 20.47 ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 OD1 ASN B 93 41.362 3.160 89.239 1.00 22.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 25.16 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3776 CA VAL B 95 32.376 10.393 88.742 1.00 27.14 ATOM 3778 CG1 VAL B 95 32.376 10.393 88.742 1.00 27.59 ATOM 3778 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 36.729 11.647 84.865 1.00 25.90 ATOM 3783 CA SER B 96 36.729 11.647 84.865 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B | | | | | | | | | 90.997 | | |
| ATOM 3760 N ASN B 93 40.314 5.677 91.017 1.00 18.85 ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 39.165 4.033 89.664 1.00 23.90 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3766 N D2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 22.60 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3778 CG1 VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 CG SER B 96 34.708 10.699 85.871 1.00 22.60 ATOM 3783 CA SER B 96 34.708 10.699 85.871 1.00 22.60 ATOM 3783 CA SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36. | | | | | | | | 6.260 | 89.962 | 1.00 | 20.47 |
| ATOM 3761 CA ASN B 93 39.534 5.509 89.795 1.00 21.96 ATOM 3762 CB ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 OD1 ASN B 93 41.362 3.160 89.239 1.00 22.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 27.59 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 34.708 10.699 85.871 1.00 25.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 | | | | | | | | 5.677 | 91.017 | 1.00 | 18.85 |
| ATOM 3762 CB ASN B 93 | | | | | | | | | 89.795 | 1.00 | 21.96 |
| ATOM 3763 CG ASN B 93 40.351 3.120 89.943 1.00 24.78 ATOM 3764 OD1 ASN B 93 41.362 3.160 89.239 1.00 22.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.595 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 25.90 ATOM 3783 CA SER B 96 34.708 10.699 85.871 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | | | | | | 89.664 | 1.00 | 23.90 |
| ATOM 3764 OD1 ASN B 93 41.362 3.160 89.239 1.00 22.35 ATOM 3765 ND2 ASN B 93 40.240 2.311 90.987 1.00 13.35 ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 37.373 8.676 90.024 1.00 24.59 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3773 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.376 N SER B 96 34.912 10.861 87.175 1.00 27.59 ATOM 3778 CG1 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3778 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 25.25 ATOM 3783 CA SER B 96 34.708 10.699 85.871 1.00 25.90 ATOM 3783 CA SER B 96 36.729 11.647 84.868 1.00 24.82 ATOM 3783 CA SER B 96 36.729 11.6647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 | | | | | | | | | 89.943 | 1.00 | 24.78 |
| ATOM 3765 ND2 ASN B 93 | | | | | | | | | | 1.00 | 22.35 |
| ATOM 3766 C ASN B 93 38.285 6.362 89.944 1.00 25.16 ATOM 3766 C ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 37.373 8.676 90.024 1.00 24.59 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 25.94 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3776 CA VAL B 95 33.035 10.393 88.742 1.00 23.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 36.729 11.647 84.868 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.6647 84.8650 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.6648 84.229 1.00 23.90 ATOM 3784 CB SER B 96 36.729 11.6648 84.229 1.00 23.90 ATOM 3784 CB SER B 96 36.729 11.6648 84.229 1.00 23.90 ATOM 3784 CB SER B 96 36.729 11.6648 84.229 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.6648 84.229 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 1.00 23.990 ATOM 3784 CB SER B 96 36.729 11.705 84.820 | MOTA | | | | | | | | | 1.00 | 13.35 |
| ATOM 3767 O ASN B 93 37.183 5.843 90.121 1.00 20.91 ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3775 C PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 36.729 11.647 84.868 1.00 24.82 ATOM 3783 CA SER B 96 36.729 11.647 84.8650 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.647 84.8650 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.648 84.229 1.00 23.99 | ATOM | | | | | | | | | 1.00 | 25.16 |
| ATOM 3768 N PRO B 94 38.449 7.693 89.887 1.00 26.37 ATOM 3769 CD PRO B 94 39.738 8.389 89.716 1.00 19.35 ATOM 3770 CA PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 25.94 ATOM 3776 CA VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 23.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3780 C VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.229 1.00 23.99 | MOTA | | | | - | | | | | | |
| ATCM 3768 N PRO B 94 39.738 8.389 89.716 1.00 19.35 ATCM 3770 CA PRO B 94 37.373 8.676 90.024 1.00 24.59 ATCM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATCM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATCM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATCM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATCM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATCM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATCM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 23.75 ATCM 3779 CG2 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATCM 3780 C VAL B 95 32.378 9.346 89.622 1.00 27.59 ATCM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATCM 3781 O VAL B 95 34.708 10.699 85.871 1.00 25.25 ATCM 3782 N SER B 96 34.708 10.699 85.871 1.00 25.90 ATCM 3783 CA SER B 96 36.729 11.647 84.868 1.00 24.82 ATCM 3783 CA SER B 96 36.729 11.647 84.868 1.00 25.90 ATCM 3784 CB SER B 96 36.729 11.0548 84.229 1.00 25.90 ATCM 3784 CB SER B 96 36.729 11.0548 84.229 1.00 25.90 ATCM 3784 CB SER B 96 36.729 11.0548 84.229 1.00 25.90 ATCM 3784 CB SER B 96 36.729 11.0548 84.229 1.00 25.90 ATCM 3784 CB SER B 96 36.729 11.0548 84.229 1.00 23.99 | MOTA | | | | | | | | | | |
| ATOM 3770 CA PRO B 94 37.373 8.676 90.024 1.00 24.59 ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.97 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 25.97 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 34.708 10.699 85.871 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 25.90 ATOM 3783 CA SER B 96 36.729 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.667 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.0548 84.229 1.00 23.99 | ATCM | | | | | | | | | | |
| ATOM 3771 CB PRO B 94 38.147 9.972 90.200 1.00 25.95 ATOM 3772 CG PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 23.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | ATOM | 3769 | CD | | - | | | | | | |
| ATOM 3771 CB PRO B 94 39.297 9.740 89.223 1.00 22.60 ATOM 3773 C PRO B 94 36.384 8.777 88.873 1.00 28.74 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 23.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 34.708 10.699 85.871 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.647 84.8650 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 | ATOM | 3770 | | | | - | | | | | |
| ATOM 3772 CG PRO B 94 36.384 8.777 888.873 1.00 28.74 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | 3 771 | CB | | | | | | | 1.00 | 22 60 |
| ATOM 3773 C PRO B 94 36.384 8.777 87.808 1.00 25.77 ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 23.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | 3772 | CG | PRO B | 94 | | | | | | |
| ATOM 3774 O PRO B 94 36.562 8.176 87.808 1.00 25.77 ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 23.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 32.378 9.346 87.175 1.00 25.69 ATOM 3781 O VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | 3773 | С | PRO B | 94 | | | | | | |
| ATOM 3775 N VAL B 95 35.332 9.553 89.112 1.00 27.14 ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 | | | 0 | PRO B | 94 | | | | | | |
| ATOM 3776 CA VAL B 95 34.317 9.812 88.103 1.00 25.94 ATOM 3777 CB VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 23.99 | | | N | VAL B | 95 | 3 | 5.332 | | | | |
| ATOM 3777 CB VAL B 95 33.035 10.393 88.742 1.00 25.75 ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 ATOM 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | VAL B | 95 | 3 | 4.317 | | | | |
| ATOM 3778 CG1 VAL B 95 32.067 10.855 87.662 1.00 26.34 87.070 3779 CG2 VAL B 95 32.376 9.346 89.622 1.00 27.59 87.00 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 87.00 3781 0 VAL B 95 35.564 11.793 87.641 1.00 25.25 870 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 870 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 870 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 870 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | VAL B | 95 | 3 | 3.035 | 10.393 | | 1.00 | 23.75 |
| ATOM 3779 CG2 VAL B 95 32.378 9.346 89.622 1.00 27.59 ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.99 | | _ | | | | | | | | 1.00 | 26.34 |
| ATOM 3780 C VAL B 95 34.912 10.861 87.175 1.00 25.69 ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | | | | | 9.346 | | 1.00 | 27.59 |
| ATOM 3781 O VAL B 95 35.564 11.793 87.641 1.00 25.25 ATOM 3782 N SER B 96 34.708 10.699 85.871 1.00 28.02 ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | atom | | | | | | | | | 1.00 | 25.69 |
| ATOM 3781 O VAB 2 33 34.708 10.699 85.871 1.00 28.02 ATOM 3782 N SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | | | | | | 87.641 | 1.00 | 25.25 |
| ATOM 3783 CA SER B 96 35.199 11.647 84.868 1.00 24.82 ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | | | | | 10.699 | | 1.00 | 28.02 |
| ATOM 3784 CB SER B 96 36.729 11.705 84.850 1.00 25.90 | | | | | | _ | | 11.647 | | 1.00 | 24.82 |
| ATOM 3784 CB SER D 36 3774 10 548 84.229 1 00 23.99 | ATOM | | | | | | | | | 1.00 | 25.90 |
| 2TOM 3785 OG SER B 96 37.2/4 10.540 | ATOM | | | | | 3 | 7 774 | | | 1.00 | 23.99 |
| | | 3785 | OG | SER B | 96 | 3 | 1.214 | 10.540 | | | , |

| ATOM | 378 | 6 C SER B 96 | 34.726 | 11,127 | 83.519 | 1.00 26,22 |
|--------------|--------------|-----------------------------|------------------|------------------|------------------|--------------------------|
| ATOM | | | 33.943 | 10.174 | 83.462 | |
| ATOM | | | 35.195 | 11.744 | 82.438 | 1.00 22.83 |
| ATOM | | | 34.818 | 11.279 | 81.110 | 1.00 28.59 |
| ATOM | 3790 | | 34.536 | 12.452 | 80.165 | 1.00 31.45 |
| ATOM | 3792 | | 33.279 | 13.203 | 80.548 | 1.00 35.09 |
| ATOM | 3792 | | 33.316 | 14.239 | 81.480 | 1.00 32.87 |
| ATOM | 3793 | | 32.148 | 14.863 | 81.911 | 1.00 37.73 |
| MOTA MOTA | 3794 3795 | | 32.036 | 12.812 | 80.049 | 1.00 34.85 |
| ATOM | 3796 | | 30.858 | 13.430 | 80.475 | 1.00 38.61 |
| ATOM | 3797 | | 30.924 29.768 | 14.453 | 81.408 | 1.00 39.45 |
| ATOM | 3798 | | 35.883 | 15.047 10.354 | 81.852 80.534 | 1.00 35.36 |
| ATOM | 3799 | | 35.859 | 9.992 | 79.358 | 1.00 28.93 1.00 28.26 |
| ATOM | 3800 | | 36.822 | 9.968 | 81.385 | |
| ATOM | 3801 | | 37.866 | 9.044 | 80.980 | 1.00 26.88 |
| ATOM | 3802 | | 39.167 | 9.369 | 81.692 | 1.00 27.99 |
| MOTA | 3803 | C ALA B 98 | 37.395 | 7.657 | 81.382 | 1.00 22.53 |
| MOTA | 3804 | O ALA B 98 | 37.721 | 6.675 | 80.722 | 1.00 21.98 |
| ATOM | 3805 | | 36.603 | 7.595 | 82.453 | 1.00 23.51 |
| MOTA | 3806 | | 36.106 | 6.326 | 82.986 | 1.00 26.36 |
| ATOM | 3807 | CB MET B 99 | 35.179 | 6.568 | 84.185 | 1.00 24.05 |
| ATOM | 3808 | CG MET B 99 | 33.822 | 7.188 | 83.875 | 1.00 28.37 |
| ATOM | 3809 3810 | SD MET B 99 | 32.966 | 7.704 | 85.406 | |
| ATOM ATOM | 3811 | CE MET B 99 C MET B 99 | 33.106 35.430 | 6.227 | 86.409 | 1.00 22.12 |
| ATOM | 3812 | O MET B 99 | 35.544 | 5.435 4.212 | 81.953 | 1.00 25.76 |
| ATOM | 3813 | N PHE B 100 | 34.724 | 6.027 | 82.031 80.992 | 1.00 26.11 1.00 22.17 |
| ATOM | 3814 | CA PHE B 100 | 34.107 | 5.222 | 79.940 | 1.00 22.17 |
| ATOM | 3815 | CB PHE B 100 | 32.582 | 5.133 | 80.088 | 1.00 22.01 |
| MOTA | 3816 | CG PHE B 100 | 31.947 | 4.254 | 79.038 | 1.00 24.22 |
| MOTA | 3817 | CD1 PHE B 100 | 32.143 | 2.872 | 79.061 | 1.00 26.61 |
| MOTA | 3818 | CD2 PHE B 100 | 31.280 | 4.813 | 77.953 | 1.00 21.22 |
| ATOM | 3819 | CE1 PHE B 100 | 31.691 | 2.059 | 78.012 | 1.00 26.91 |
| MOTA | 3820 | CE2 PHE B 100 | 30.825 | 4.010 | 76.894 | 1.00 24.80 |
| ATOM ATOM | 3821 3822 | CZ PHE B 100 C PHE B 100 | 31.033 | 2.632 | 76.924 | 1.00 24.85 |
| ATOM | 3823 | O PHE B 100 | 34.425 | 5.695 | 78.514 | 1.00 24.86 |
| ATOM | 3824 | N THR B 101 | 34.922 34.131 | 4.920 6.957 | 77.694 78.204 | 1.00 21.40 |
| ATOM | 3825 | CA THR B 101 | 34.390 | 7.469 | 76.854 | 1.00 24.24 1.00 24.54 |
| ATOM | 3826 | CB THR B 101 | 33.914 | 8.926 | 76.708 | 1.00 24.46 |
| MOTA | 3827 | OG1 THR B 101 | 32.504 | 8.985 | 76.953 | 1.00 27.64 |
| ATOM | 3828 | CG2 THR B 101 | 34.191 | 9.445 | 75.297 | 1.00 22.19 |
| ATOM | 3829 | C THR B 101 | 35.872 | 7.387 | 76.483 | 1.00 25.26 |
| ATOM | 3830 | O THR B 101 | 36.231 | 6.856 | 75.430 | 1.00 25.47 |
| ATOM | 3831 | N GLY B 102 | 36.725 | 7.916 | 77.350 | 1.00 23.74 |
| MOTA | 3832 3833 | CA GLY B 102 | 38.153 | 7.867 | 77.096 | 1.00 24.53 |
| ATOM ATOM | 3834 | C GLY B 102 O GLY B 102 | 38.657 | 6.434 | 77.046 | 1.00 24.06 |
| ATOM | 3835 | N SER B 103 | 39.346 | 6.045 | 76.100 | 1.00 22.53 |
| ATOM | 3836 | CA SER B 103 | 38.316 38.730 | 5.651 4.253 | 78.067 78.146 | 1.00 22.02 |
| ATOM | 3837 | CB SER B 103 | 38.193 | 3.613 | 79.427 | 1.00 20.45 |
| ATOM | 3838 | OG SER B 103 | 38.820 | 4.166 | 80.567 | 1.00 26.48 |
| MOTA | 3839 | C SER B 103 | 38.268 | 3.446 | 76.938 | 1.00 20.53 |
| ATOM | 3840 | O SER B 103 | 39.034 | 2.669 | 76.372 | 1.00 16.82 |
| ATOM | 3841 | N SER B 104 | 37.014 | 3.642 | 76.542 | 1.00 17.11 |
| ATOM | 3842 | CA SER B 104 | 36.462 | 2.937 | 75.395 | 1.00 23.32 |
| ATOM | 3843 | CB SER B 104 | 34.980 | 3.289 | 75.228 | 1.00 22.93 |
| MOTA | 3844 | OG SER B 104 | 34.424 | 2.557 | 74.161 | 1.00 24.75 |
| ATOM | 3845 | C SER B 104 | 37.221 | 3.288 | 74.116 | 1.00 21.97 |
| MOTA | 3546 | O SER B 104 | 37.451 | 2.434 | 73.256 | 1.00 22.83 |
| ATOM ATOM | 3847 3848 | N LEU B 105 CA LEU B 105 | 37.619 38.354 | 4.549 | 73.997 | 1.00 23.00 |
| ATOM ATOM | 3849 | CB LEU B 105 | 38.354 38.443 | 5.007 | 72.825 | 1.00 25.12 |
| ATOM | 3850 | CG LEU B 105 | 38.702 | 6.536 7.289 | 72.859 71.553 | 1.00 29.25 1.00 34.27 |
| ATOM | 3851 | CD1 LEU B 105 | 37.662 | 6.888 | 70.512 | 1.00 34.27 |
| | | | | J. J. J. J | | JT |

| | | | | | | | | ma 010 | 1 00 34 30 |
|--------|--------|-----|-------|-------|---|--------|--------|--------|------------|
| MOTA | 3852 | CD2 | LEU B | 105 | | 38.629 | 8.802 | 71.819 | 1.00 34.30 |
| | 3853 | С | LEU B | | | 39.755 | 4.374 | 72.813 | 1.00 27.39 |
| ATOM | | ō | LEU B | | | 40.262 | 3.955 | 71.765 | 1.00 20.15 |
| ATOM | 3854 | | | | | 40.371 | 4.293 | 73.988 | 1.00 23.62 |
| ATOM | 3855 | N | ALA B | | | | | | 1.00 22.73 |
| ATOM | 3856 | CA | ALA B | 106 | | 41.704 | 3.692 | 74.115 | |
| ATOM | 3857 | CB | ALA B | 106 | | 42.263 | 3.939 | 75.529 | 1.00 17.46 |
| | | | ALA B | | | 41.639 | 2.189 | 73.846 | 1.00 22.77 |
| ATOM | 3858 | C | | | | 42.583 | 1.597 | 73.316 | 1.00 24.98 |
| MOTA | 3859 | 0 | ALA B | | | | | | 1.00 23.54 |
| ATOM | 3860 | N | THR B | 107 | | 40.523 | 1.567 | 74.224 | |
| MOTA | 3861 | CA | THR B | 107 | | 40.355 | 0.132 | 74.033 | 1.00 19.76 |
| | 3862 | СВ | THR B | | | 39.236 | -0.410 | 74.947 | 1.00 22.85 |
| MOTA | | | THR B | | | 39.572 | -0.128 | 76.306 | 1.00 16.29 |
| MOTA | 3863 | OG1 | | | | | -1.917 | 74.787 | 1.00 17.21 |
| ATOM | 3864 | CG2 | THR B | | | 39.085 | | | 1.00 23.47 |
| MOTA | 3865 | С | THR B | 107 | | 40.036 | -0.169 | 72.571 | |
| ATOM | 3866 | 0 | THR B | 107 | | 40.540 | -1.138 | 72.001 | 1.00 19.25 |
| | 3867 | N | GLY B | 108 | | 39.191 | 0.656 | 71.959 | 1.00 24.87 |
| MOTA | | | | | | 38.879 | 0.434 | 70.560 | 1.00 21.32 |
| MOTA | 3868 | CA | GLY B | | | | 0.594 | 69.757 | 1.00 22.01 |
| MOTA | 3869 | C | GLY B | | | 40.161 | | 60.761 | 1.00 20.46 |
| ATOM | 3870 | 0 | GLY B | 108 | | 40.388 | -0.099 | 68.761 | |
| | 3871 | N | SER B | 109 | | 41.018 | 1.508 | 70.197 | 1.00 19.89 |
| MOTA | | CA | SER B | | | 42.274 | 1.749 | 69.499 | 1.00 19.37 |
| MOTA | 3872 | | | | | 42.993 | 2.956 | 70.107 | 1.00 18.28 |
| MOTA | 3873 | CB | SER B | | | | 4.145 | 69.882 | 1.00 21.29 |
| MOTA | 3874 | 0G | SER B | | | 42.250 | | | 1.00 20.70 |
| ATOM | 3875 | С | SER B | 109 | | 43.168 | 0.513 | 69.542 | |
| ATOM | 3876 | 0 | SER B | 109 | | 43.940 | 0.261 | 68.617 | 1.00 20.69 |
| | 3877 | N | THR B | | | 43.065 | -0.259 | 70.616 | 1.00 20.54 |
| MOTA | | | | | | 43.858 | -1.475 | 70.729 | 1.00 19.98 |
| MOTA | 3878 | CA | THR B | | | | -2.043 | 72.158 | 1.00 20.63 |
| ATOM | 3879 | CB | THR B | | • | 43.826 | | | 1.00 20.72 |
| MOTA | 3880 | OG1 | THR E | 110 | | 44.632 | -1.215 | 73.007 | |
| ATOM | 3881 | CG2 | THR E | 110 | | 44.371 | -3.470 | 72.188 | 1.00 20.05 |
| | 3882 | C | THR E | | | 43.333 | -2.507 | 69.738 | 1.00 21.61 |
| ATOM | | | | | | 44.115 | -3.239 | 69.127 | 1.00 18.11 |
| MOTA | 3883 | 0 | THR E | | | | -2.557 | 69.567 | 1.00 18.29 |
| ATOM | 3884 | N | VAL E | | | 42.012 | | | 1.00 20.36 |
| ATOM | 3885 | CA | VAL E | 111 | | 41.432 | -3:486 | 68.608 | |
| ATOM | 3886 | CB | VAL E | 111 | | 39.886 | -3.494 | 68.677 | 1.00 23.94 |
| | 3887 | | VAL E | | | 39.324 | -4.442 | 67.619 | 1.00 24.37 |
| ATOM | | | VAL E | | | 39.426 | -3.937 | 70.063 | 1.00 21.60 |
| ATOM | 3888 | | | | | 41.872 | -3.080 | 67.197 | 1.00 20.35 |
| ATOM | 3889 | С | VAL E | | | | | 66.362 | 1.00 23.29 |
| MOTA | 3890 | 0 | VAL E | | | 42.146 | -3.936 | | 1.00 22.07 |
| ATOM . | 3891 | N | GLN E | 3 112 | | 41.953 | -1.775 | 66.937 | |
| | 3892 | CA | GLN E | 112 | | 42.367 | -1.290 | 65.617 | 1.00 22.34 |
| MOTA | | CB | GLN E | | | 42.199 | 0.230 | 65.513 | 1.00 24.54 |
| MOTA | 3893 | | GLN E | | | 40.810 | 0.729 | 65.843 | 1.00 20.63 |
| MOTA | 3894 | CG | | | | | 2.236 | 65.742 | 1.00 21.19 |
| MOTA | 3895 | CD | GLN E | | | 40.700 | | 64.645 | 1.00 26.73 |
| MOTA | 3896 | OEl | GLN E | 3 112 | | 40.664 | 2.794 | | |
| ATOM | 3897 | NE2 | GLN E | 112 | | 40.667 | 2.905 | 66.886 | 1.00 18.33 |
| | 3898 | c | GLN E | | | 43.826 | -1.635 | 65.363 | 1.00 23. 1 |
| ATOM | | | GLN E | | | 44.195 | -2.020 | 64.257 | 1.00 15.79 |
| ATOM | 3899 | 0 | | | | 44.660 | -1.476 | 66.389 | 1.00 20.60 |
| MOTA | 3900 | N | ALA E | | | | | 66.249 | 1.00 18.02 |
| ATOM | 3901 | CA | ALA E | | | 46.070 | -1.790 | | 1.00 20.84 |
| MOTA | 3902 | CB | ALA E | 3 113 | | 46.794 | -1.536 | 67.548 | 1.00 20.54 |
| | 3903 | C | ALA E | 3 113 | | 46.170 | _3.262 | 65.863 | 1.00 23.78 |
| MOTA | | | ALA I | 1113 | | 46.982 | -3.642 | 65.023 | 1.00 19.83 |
| MOTA | 3904 | 0 | | | | 45.331 | -4.091 | 66.477 | 1.00 21.45 |
| ATOM | . 3905 | N | ILE E | | | | | 66.168 | 1.00 24.26 |
| ATOM | 3906 | CA | ILE F | 3 114 | | 45.344 | -5.511 | | 1.00 20.72 |
| | 3907 | CB | ILE E | 3 114 | | 44.507 | -6.306 | 67.191 | |
| ATOM | 3908 | CG2 | ILE E | | | 44.476 | -7.779 | 66.800 | 1.00 21.92 |
| ATOM | | | ILE F | | | 45.116 | -6.144 | 68.593 | 1.00 24.32 |
| ATOM | 3909 | CG1 | | | | | -6.872 | 69.694 | 1.00 19.01 |
| ATOM | 3910 | CDI | | | | 44.364 | | 54.753 | 1.00 26.75 |
| ATOM | 3911 | С | ILE E | | | 44.808 | -5.765 | | |
| | 3912 | ō | ILE E | 3 114 | | 45.305 | -6.640 | 64.032 | 1.00 20.18 |
| ATOM | | N | GLU I | 3 115 | | 43.792 | -5.009 | 64.347 | 1.00 24.59 |
| ATOM | 3913 | | GLU I | 115 | | 43.243 | ~5.198 | 63.005 | 1.00 29.26 |
| ATOM | 3914 | CA | GIO I | , 115 | | | _ | 62.770 | |
| ATOM | 3915 | CB | GLU I | 2 TT2 | | 42.043 | -4.278 | 63.800 | |
| ATCM | 3916 | CG | GLU 1 | 8 115 | | 40.940 | -4.421 | | |
| | 3917 | CD | GLU I | B 115 | | 39.757 | -3.519 | 63.516 | T.00 20.74 |
| ATOM | J | | | | | | | | |

Figure 18-60

| MOTA | 3918 | 3 OE1 GLU B 115 | 39.980 | -2.374 | 63.072 | 1.00 40.63 |
|--------------|------|-----------------|------------------|---------|--------|------------|
| MOTA | 3919 | 9 OE2 GLU B 115 | | | | 1.00 39.86 |
| ATOM | 3920 | | | | 61.974 | 1.00 31.52 |
| MOTA | 3921 | | | | | |
| ATOM | 3922 | | | | 60.964 | 1.00 26.43 |
| ATOM | 3923 | | | | 62.234 | 1.00 26.04 |
| ATOM | 3924 | | | | 61.324 | 1.00 26.21 |
| | | | | | 61.775 | 1.00 23.21 |
| MOTA | 3925 | | | | 61.601 | 1.00 23.82 |
| ATOM | 3926 | | | | 60.163 | 1.00 31.43 |
| MOTA | 3927 | | | | 59.253 | 1.00 26.45 |
| MOTA | 3928 | | | -0.771 | 59.945 | 1.00 24.59 |
| MOTA | 3929 | | | -4.644 | 61.243 | 1.00 28.60 |
| MOTA | 3930 | | 47.857 | -4.884 | 60.189 | 1.00 25.01 |
| MOTA | 3931 | N PHE B 117 | 47.470 | -5.324 | 62.363 | 1.00 26.22 |
| ATOM | 3932 | CA PHE B 117 | 48.421 | -6.425 | 62.400 | 1.00 28.05 |
| MOTA | 3933 | CB PHE B 117 | 48.516 | | 63.805 | 1.00 32.15 |
| MOTA | 3934 | CG PHE B 117 | | | 63.869 | 1.00 33.88 |
| MOTA | 3935 | | | -8.321 | 63.713 | 1.00 33.52 |
| ATOM | 3936 | | | -9.502 | 64.054 | 1.00 33.32 |
| ATOM | 3937 | | | -9.521 | 63.740 | 1.00 32.83 |
| MOTA | 3938 | | | -10.710 | | |
| MOTA | 3939 | CZ PHE B 117 | 50.674 | -10.717 | 64.082 | 1.00 35.69 |
| MOTA | 3940 | C PHE B 117 | 47.929 | | 63.926 | 1.00 36.72 |
| ATOM | 3941 | O PHE B 117 | | -7.508 | 61.456 | 1.00 26.43 |
| ATOM | 3942 | N LEU B 118 | 48.689 | -8.061 | 60.669 | 1.00 27.61 |
| ATOM | 3943 | | 46.642 | -7.809 | 61.551 | 1.00 23.59 |
| ATOM | 3944 | CA LEU B 118 | 46.048 | -8.820 | 60.705 | 1.00 29.15 |
| | | CB LEU B 118 | 44.585 | -9.039 | 61.099 | 1.00 28.78 |
| ATOM | 3945 | CG LEU B 118 | 44.375 | -9.478 | 62.557 | 1.00 35.24 |
| ATOM | 3946 | CD1 LEU B 118 | 42.898 | -9.763 | 62.788 | 1.00 31.92 |
| MOTA | 3947 | CD2 LEU B 118 | | -10.723 | 62.856 | 1.00 33.40 |
| MOTA | 3948 | C LEU B 118 | 46.153 | -8.422 | 59.236 | 1.00 30.15 |
| MOTA | 3949 | O LEU B 118 | 46.350 | -9.276 | 58.379 | 1.00 27.04 |
| ATOM | 3950 | N LYS B 119 | 46.035 | -7.128 | 58.947 | 1.00 27.96 |
| ATOM | 3951 | CA LYS B 119 | 46.127 | -6.663 | 57.569 | 1.00 26.69 |
| ATOM | 3952 | CB LYS B 119 | 45.470 | -5.291 | 57.412 | 1.00 23.94 |
| MOTA | 3953 | CG LYS B 119 | 43.998 | -5.260 | 57.795 | 1.00 24.41 |
| ATOM | 3954 | CD LYS B 119 | 43.327 | -3.970 | 57.350 | 1.00 27.53 |
| ATOM | 3955 | CE LYS B 119 | 44.024 | -2.739 | 57.886 | 1.00 33.13 |
| MOTA | 3956 | NZ LYS B 119 | 43.371 | -1.479 | 57.428 | 1.00 27.75 |
| MOTA | 3957 | C LYS B 119 | 47.57 7 | -6.598 | 57.101 | 1.00 29.12 |
| ATOM | 3958 | O LYS B 119 | 47.864 | -6.160 | 55.984 | 1.00 35.25 |
| ATOM | 3959 | N GLY B 120 | 48.493 | -7.034 | 57.958 | 1.00 30.25 |
| MOTA | 3960 | CA GLY B 120 | 49.896 | -7.037 | 57.585 | 1.00 28.38 |
| ATOM | 3961 | C GLY B 120 | 50.642 | -5.751 | 57.861 | 1.00 27.91 |
| MOTA | 3962 | O GLY B 120 | 51.775 | -5.582 | 57.403 | 1.00 22.25 |
| ATOM | 3963 | N ASN B :21 | 50.024 | -4.836 | 58.600 | 1.00 25.42 |
| MOTA | 3964 | CA ASN B . 21 | 50.695 | | 58.919 | 1.00 29.49 |
| MOTA | 3965 | CB ASN B 121 | 49.758 | -2.389 | 58.727 | 1.00 30.07 |
| ATOM | 3966 | CG ASN B 121 | 49.201 | -2.307 | 57.325 | 1.00 32.25 |
| MOTA | 3967 | OD1 ASN B 121 | 49.924 | -2.491 | 56.350 | 1.00 35.44 |
| ATOM | 3968 | ND2 ASN B 121 | | -2.006 | 57.217 | |
| MOTA | 3969 | C ASN B 121 | 51.172 | -3.637 | 60.361 | 1.00 30.92 |
| ATOM. | 3970 | O ASN B 121 | 50.971 | -4.631 | 61.059 | 1.00 27.08 |
| ATOM | 3971 | N VAL B 122 | 51.810 | -2.560 | 60.796 | 1.00 28.46 |
| ATOM | 3972 | CA VAL B 122 | 52.309 | -2.457 | 62.155 | 1.00 29.48 |
| ATOM | 3973 | CB VAL B 122 | 53.840 | -2.352 | 62.177 | |
| ATOM | 3974 | CG1 VAL B 122 | 54.334 | | | |
| | 3975 | CG2 VAL B 122 | | -2.294 | 63.611 | 1.00 32.22 |
| ATOM ATOM | 3976 | C VAL B 122 | 54.446 51 713 | -3.544 | 61.458 | 1.00 33.57 |
| | | | 51.713 | -1.196 | 62.748 | 1.00 29.04 |
| ATOM | 3977 | | 51.800 | -0.118 | 62.153 | 1.00 27.47 |
| ATOM | 3978 | N ALA B 123 | 51.100 | -1.326 | 63.918 | 1.00 26.71 |
| MOTA | 3979 | CA ALA B 123 | 50.477 | -0.177 | 64.559 | 1.00.25.62 |
| MOTA | 3980 | CB ALA B 123 | 48.963 | -0.281 | 64.447 | 1.00 21.65 |
| ATOM | 3981 | C ALA B 123 | 50.872 | -0.005 | 66.017 | 1.00 28.62 |
| ATOM | 3982 | 0 ALA B 123 | 51.227 | -0.965 | 66.712 | 1.00 26.96 |
| MOTA | 3983 | N PHE B 124 | 50.805 | 1.239 | 66.472 | 1.00 22.85 |



| MOTA MOTA ATOM | 3984 3985 3986 3987 | CB CG | PHE B 124 PHE B 124 PHE B 124 PHE B 124 | 51.122 52.419 52.762 52.533 | 1.577 2.404 3.000 2.304 | 67.876 69.225 70.403 | 1.00 17.31 1.00 16.88 1.00 18.52 1.00 17.52 1.00 17.88 |
|----------------------|------------------------------|-----------|--|--------------------------------------|----------------------------------|----------------------------|--|
| MOTA MOTA | 3988 | | PHE B 124 | 53.382 | 4.245 | | 1.00 17.33 |
| ATOM ATOM | 3989 | CE1 | PHE B 124. | 52.914 | 2.837 | | 1.00 21.97 |
| ATOM | 3990 | CE2 | PHE B 124 | 53.769 | 4.790 | | 1.00 20.16 |
| MOTA | 3991 | CZ | PHE B 124 | 53.535 | 4.084 | 71.698 68.421 | 1.00 18.77 |
| ATOM | 3992 | С | PHE B 124 | 49.937 | 2.348 3.311 | 67.820 | 1.00 16.62 |
| ATOM | 3993 | 0 | PHE B 124 | 49.462 49.418 | 1.868 | | 1.00 16.69 |
| MOTA | 3994 | N | ASN B 125 | 48.320 | 2.528 | 70.238 | 1.00 16.22 |
| MOTA | 3995 | CA | ASN B 125 ASN B 125 | 47.129 | 1.603 | 70.435 | 1.00 12.71 |
| MOTA | 3996 | CB | ASN B 125 | 46.095 | 2.209 | 71.346 | 1.00 19.79 |
| ATOM | 3997 | CG OD1 | ASN B 125 | 45.930 | 3.430 | 71.372 | 1.00 20.83 |
| MOTA | 3998 3999 | MD3 | ASN B 125 | 45.376 | 1.371 | 72.087 | 1.00 12.31 |
| MOTA | 4000 | C | ASN B 125 | 48.790 | 3.004 | 71.600 | 1.00 19.19 1.00 20.99 |
| MOTA | 4001 | ŏ | ASN B 125 | 48.687 | 2.280 | 72.585 | 1.00 20.33 |
| MOTA MOTA | 4002 | N | PRO B 126 | 49.335 | 4.226 | 71.668 70.555 | 1.00 21.39 |
| ATOM | 4003 | CD | PRO B 126 | 49.595 | 5.156 4.805 | 72.917 | 1.00 21.60 |
| ATOM | 4004 | CA | PRO B 126 | 49.833 | 6.161 | 72.459 | 1.00 21.07 |
| ATOM | 4005 | CB | PRO B 126 | 50.398 49.530 | 6.487 | 71.269 | 1.00 17.70 |
| MOTA | 4006 | CG | PRO B 126 PRO B 126 | 48.808 | 4.942 | 74.034 | 1.00 20.69 |
| ATOM | 4007 | C | PRO B 126 | 49.178 | 5.053 | 75.198 | 1.00 19.79 |
| MOTA | 4008 | O N | ALA B 127 | 47.525 | 4.937 | 73.689 | 1.00 16.67 |
| ATOM | 4009 4010 | CA | ALA B 127 | 46.476 | 5.065 | 74.698 | 1.00 20.44 1.00 19.56 |
| ATOM | 4011 | CB | ALA B 127 | 45.198 | 5.609 | 74.066 | 1.00 20.80 |
| ATOM ATOM | 4012 | Ċ | ALA B 127 | 46.169 | 3.747 3.742 | 75.401 76.472 | 1.00 19.47 |
| ATOM | 4013 | 0 | ALA B 127 | 45.555 | 2.634 | 74.800 | 1.00 20.52 |
| ATOM | 4014 | N | GLY B 128 | 46.587 46.325 | 1.333 | 75.399 | 1.00 19.43 |
| ATOM | 4015 | CA | GLY B 128 | 47.327 | 0.910 | 76.463 | 1.00 20.56 |
| MOTA | 4016 | С | GLY B 128 GLY B 128 | 48.182 | 1.697 | 76.869 | 1.00 18.37 |
| ATOM | 4017 | 0 | GLY B 129 | 47.215 | -0.333 | 76.929 | 1.00 19.68 |
| MOTA | 4018 4019 | N CA | GLY B 129 | 48.136 | -0.820 | 77.943 | 1.00 19.93 1.00 25.25 |
| MOTA | 4020 | c | GLY B 129 | 47.620 | -0.619 | | 1.00 23.23 |
| atom atom | 4021 | ō | GLY B 129 | 48.383 | -0.686 | | 1.00 16.04 |
| ATOM | 4022 | N | MET B 130 | 46.317 | -0.374 -0.161 | | 1.00 19.26 |
| MOTA | 4023 | CA | MET B 130 | 45.677 44.301 | 0.451 | | 1.00 17.94 |
| ATOM | 4024 | CB | MET B 130 MET B 130 | 44.413 | 1.728 | 79.653 | 1.00 22.95 |
| ATOM | 4025 | CG | MET B 130 | 42.873 | 2.615 | 79.307 | 1.00 31.83 |
| ATOM | 4026 | SD CE | MET B 130 | 41.957 | 1.358 | 78.382 | 1.00 20.22 1.00 22.63 |
| ATOM | 4027 4028 | | MET B 130 | 45.598 | -1.548 | | 1.00 22.03 |
| ATOM | 4029 | .0 | MET B 130 | 44.546 | -2.173 | | |
| atom atom | 4030 | | HIS B 131 | 46.737 | -1.999 | | |
| ATOM | 4031 | CA | HIS B 131 | 46.853 | -3.343 -3.804 | | 1.00 17.61 |
| ATOM | 4032 | | HIS B 131 | 48.323 49.316 | -2.979 | | 1.00 14.01 |
| TOM | 4033 | CG | HIS B 131 | 49.138 | -1.904 | 83.915 | 1.00 13.47 |
| atom | 4034 | | 2 HIS B 131 1 HIS B 131 | 50.680 | -3.190 |) 83.051 | 1.00 18.00 |
| ATOM | 4035 | | 1 HIS B 131 | 51.297 | -2.283 | 1 83.789 | |
| ATOM | 4036 4037 | | 2 HIS B 131 | 50.384 | -1.48 | | |
| ATOM | 4038 | | HIS B 131 | 46.329 | -3.72 | 4 83.852 | |
| ATOM | 4039 | | HIS B 131 | 46.452 | -4.88 | 3 84.236 4 84.586 | |
| atom atom | 4040 | | HIS B 132 | 45.721 | -2.79 -3.11 | | 1.00 20.87 |
| ATOM | 4041 | | HIS B 132 | 45.241 | -1.93 | | 1.00 18.85 |
| ATOM | 4042 | | HIS B 132 | 45.513 46.966 | | | 1.00 20.00 |
| ATOM | 4043 | CG | HIS B 132 | 45.960 | | | 1.00 15.74 |
| ATOM | 1044 | | 2 HIS B 132 | 47.810 | -2.65 | 5 87.659 | 9 1.00 14.72 |
| LTOM | 4045 | | 1 HIS B 132 1 HIS B 132 | 49.014 | -2.13 | 9 87.83 | |
| ATOM | 4046 | | 2 HIS B 132 | 48.984 | -0.87 | 2 87.46 | |
| ATOM | 404.7 4048 | | HIS B 132 | 43.778 | -3.54 | | |
| =TOM | 4049 | _ | HIS B 132 | 43.478 | -4.29 | 8 87.07 | u 1.00 ±02 |
| RTOM | , , , , , | | A 1120 | | /BAIR = | 001 | |

4050

178/263 Figure 18-62,

MOTA 85.271 ALA B 133 42.878 -3.088 1.00 16.54 ATOM 4051 CA ALA B 133 41.457 ~3.396 85.424 1.00 19.13 4052 MOTA CB ALA B 133 40.654 -2.70484.328 1.00 23.56 4053 ATOM C ALA B 133 41.127 -4.883 85.439 1.00 23.12 ATOM 4054 0 ALA B 133 41.718 -5.677 84.696 1.00 18.03 ATOM 4055 N PHE В 40.181 134 -5.257 86.294 1.00 19.69 4056 ATOM CA PHE B 134 39.762 -6.649 86.365 1.00 19.35 ATOM 4057 PHE B 134 CB 39.583 -7.122 87.818 1.00 21.26 ATOM 4058 CG PHE В 134 40.837 -7.053 88.646 1.00 23.41 4059 CD1 PHE B 134 41.041 ATOM -6.009 89.544 1.00 24.25 4060 CD2 PHE B 134 ATOM 41.820 -8.027 1.00 22.80 88.522 ATOM 4061 CEL PHE В 134 42.207 -5.935 90.311 1.00 23.36 4062 ATOM CE2 PHE B 134 42.997 -7.964 89.283 1.00 27.74 4063 CZ PHE B 134 MOTA 43.190 -6.917 90.178 1.00 24.05 4064 С PHE B 134 -6.816 ATOM 38.444 85.621 1.00 18.60 PHE B 134 37.815 MOTA 4065 0 -5.849 85.196 1.00 13.82 4066 N LYS B 135 MOTA 38.050 -8.064 85.454 1.00 19.78 MOTA 4067 CA LYS B 135 36.813 -8.421 84.782 1.00 28.09 MOTA 4068 CB LYS B 135 36.501 -9.879 85.125 1.00 34.06 CG 4069 LYS B 135 MOTA 35.077 -10.310 84.953 1.00 42.76 ATOM 4070 CD LYS B 135 34.927 -11.745 85.437 1.00 48.44 4071 LYS B 135 ATOM CE 33.462 -12.152 85.531 1.00 55.66 4072 ΝZ LYS B 135 ATOM 32.727 -11.332 86.544 1.00 51.65 4073 LYS B 135 MOTA C 35.639 -7.512 85.172 1.00 28.27 ATOM 4074 0 LYS B 135 34.927 -6.999 84.309 1.00 24.86 4075 N SER B 136 -7.292 35.450 ATOM 86.470 1.00 29.89 4076 CA **SER B 136** ATOM 34.331 -6.477 86.933 1.00 30.86 -7.388 ATOM 4077 CB **SER B 136** 33.282 87.582 1.00 31.57 4078 OG **SER B 136** 32.916 -8.434 86.698 ATOM 1.00 45.10 4079 C SER B 136 -5.380 ATOM 34.705 87.923 1.00 31.50 **SER B 136** 4080 ATOM 0 33.887 ~4.997 88.765 1.00 24.54 MOTA 4081 N ARG B 137 35.920 -4.854 87.835 88.794 1.00 22.63 -3.826 4082 CA ARG B 137 36.291 MOTA 1.00 25.51 ARG B 137 4083 CB ATOM 36.629 -4:486 90.136 1.00 29.62 MOTA 4084 CG ARG B 137 36.391 -3.57891.318 1.00 36.21 4085 CD ARG B 137 MOTA 36.874 -4.160 92.631 1.00 40.79 4086 NE ARG B 137 -3.357 36.365 ATOM 93.744 1.00 45.95 ARG B 137 MOTA 4087 CZ36.863 -3.369 94.973 1.00 41.97 MOTA 4088 NH1 ARG B 137 37.897 -4.144 95.263 1.00 43.42 4089 ARG B NH2 137 -2.604 95.913 ATOM 36.322 1.00 46.65 4090 ARG B 137 MOTA C 37.461 -2.956 88.339 1.00 24.73 ARG B 137 MOTA 4091 0 38.420 -3.44187.734 1.00 19.32 4092 N ALA B 138 MOTA 37.372 -1.663 88.631 1.00 16.77 4093 CA ALA B 138 ATOM 38.428 -0.733 88.270 1.00 18.50 4094 CB ALA B 138 MOTA 37.939 0.694 88.401 1.00 17.24 4095 C ALA B 138 39.597 -0.964 89.216 ATOM 1.00 22.62 4096 90.346 **ALA B 138** 39 411 ATOM -1.4191.00 18.98 4097 N **ASN B 139** 40.301 88.759 ATOM -0.641 1.00 20.82 CA 4098 ASN B 139 41.989 -0.828 89.585 ATOM 1.00 25.17 4099 CB ASN B 89.689 139 42.311 -2.329 ATOM 1.00 20.59 MOTA 4100 CG ASN В 139 43.556 -2.608 90.511 1.00 27.70 OD1 4101 ASN B 43.726 MOTA 139 -2.057 91.592 1.00 22.43 4102 ND2 **ASN B 139** 44.420 90.010 ATOM -3.487 1.00 24.43 4103 C ASN B 139 43.176 -0.062 89.020 MOTA 1.00 22.37 87.799 O ASN B ATOM 4104 139 43.338 0.038 1.00 17.50 1.00 21.67 4105 N **GLY B 140** 43.984 89.920 ATOM 0.496 MOTA 4106 CA GLY B 140 45.166 89.524 1.249 1.00 23.06 4107 C GLY B 140 45.005 88.402 ATOM 2.268 1.00 26.29 4108 0 **GLY B 140** 45.827 87.479 ATOM 2.301 1.00 22.47 1.00 22.33 4109 N PHE B 141 43.958 88.473 3.093 ATOM 87.461 PHE B 141 ATOM 4110 CA 43.694 4.126 1.00 19.01 86.997 4111 CB PHE B 141 44.996 ATOM 4.806 1.00 22.90 4112 CG PHE В 141 45.810 88.097 1.00 23.17 ATOM 5.433 PHE B 141 87.842 CD1 47.114 ATON 4113 5.851 1.00 22.17 CD2 PHE B 141 4114 45.281 5.635 .89.366 1.00 23.40 ATOM 88.833 1.00 24.02 4115 CE1 PHE B 141 47.876 6.462 MOTA

| | | | | | | | 1.00 23.03 |
|--------|------|---------|----------------|--------------|----------------|---------|------------|
| ATOM | 4116 | CE2 PHE | B 141 | 46.033 | 6.244 | 90.361 | |
| | | CZ PHE | B 141 | 47.335 | 6.658 | 90.092 | 1.00 25.15 |
| MOTA | 4117 | | | 43.029 | 3.538 | 86.214 | 1.00 23.69 |
| MOTA | 4118 | | B 141 | | 4.283 | 85.335 | 1.00 18.88 |
| ATOM | 4119 | O PHE | B 141 | 42.596 | | | 1.00 15.03 |
| MOTA | 4120 | N CYS | B 142 | 42.962 | 2.211 | 86.122 | |
| | | | B 142 | 42.380 | 1.578 | 84.938 | 1.00 19.55 |
| MOTA | 4121 | | | 43.193 | 0.336 | 84.552 | 1.00 20.38 |
| MOTA | 4122 | CB CYS | | | 0.662 | 84.190 | 1.00 37.40 |
| MOTA | 4123 | SG CYS | B 142 | 44.933 | | | 1.00 22.77 |
| MOTA | 4124 | C CYS | B 142 | 40.923 | 1.171 | 85.098 | |
| | | O CYS | в 142 | 40.561 | 0.514 | 86.082 | 1.00 23.04 |
| MOTA | 4125 | 0 010 | B 143 | 40.094 | 1.557 | 84.130 | 1.00 15.24 |
| ATOM | 4126 | n tyr | B 143 | | 1.194 | 84.155 | 1.00 21.97 |
| ATOM | 4127 | CA TYR | в 143 | 38.675 | | 03.133 | 1.00 18.06 |
| MOTA | 4128 | CB TYR | в 143 | 37.795 | 2.372 | 83.723 | 1.00 10.00 |
| | | CG TYR | B 143 | 38.016 | 3.622 | 84.535 | 1.00 24.34 |
| MOTA | 4129 | | B 143 | 39.038 | 4.516 | 84.214 | 1.00 23.20 |
| MOTA | 4130 | | | 39.265 | 5.658 | 84.991 | 1.00 27.42 |
| MOTA | 4131 | | B 143 | | | 85.652 | 1.00 19.15 |
| ATOM | 4132 | CD2 TYR | B 143 | 37.226 | 3.892 | 85.652 | 1.00 21.92 |
| | 4133 | | в 143 | 37.441 | 5.023 | 86.432 | 1.00 21.92 |
| MOTA | | CO TOUR | В 143 | 38.458 | 5.900 | 86.099 | 1.00 23.94 |
| MOTA | 4134 | CZ TYR | D 143 | 38.655 | 7.015 | 86.877 | 1.00 22.37 |
| MOTA | 4135 | OH TYR | в 143 | | | 83.218 | 1.00 19.91 |
| ATOM | 4136 | C TYR | В 143 | 38.431 | 0.008 | | 1.00 22.50 |
| | 4137 | O TYR | В 143 | 37.665 | -0.902 | 83.535 | 1.00 22.30 |
| MOTA | 4138 | | В 144 | 39.083 | 0.026 | 82.061 | 1.00 19.20 |
| MOTA | | | В 144 | 38.938 | -1.055 | 81.082 | 1.00 19.68 |
| ATOM | 4139 | | | 38.282 | -0.528 | 79.787 | 1.00 20.26 |
| MOTA | 4140 | CB ILE | В 144 | | -1.649 | 78.760 | 1.00 15.37 |
| ATOM | 4141 | CG2 ILE | B 144 | 38:151 | | | 1.00 20.93 |
| | 4142 | CG1 ILE | В 144 | 36.901 | 0.053 | 80.113 | 1.00 20.33 |
| ATOM | | CD1 ILE | R 144 | 36.198 | 0.697 | 78.917 | 1.00 23.75 |
| MOTA | 4143 | | В 144 | 40.320 | -1.627 | 80.774 | 1.00 22.78 |
| MOTA | 4144 | | | 41.281 | -0.873 | 80.600 | 1.00 22.01 |
| MOTA | 4145 | - | В 144 | | | 80.723 | 1.00 23.18 |
| ATOM | 4146 | n asn | IB 145 | 40.422 | -2.956 | | 1.00 20.63 |
| | 4147 | CA ASN | B 145 | 41.698 | -3.623 | 80.451 | |
| MOTA | | | | 41.778 | -4.935 | 81.243 | 1.00 17.81 |
| MOTA | 4148 | | | 43.188 | -5.531 | 81.268 | 1.00 25.17 |
| MOTA | 4149 | CG ASN | I B 145 | | -5.742 | 80.227 | 1.00 23.63 |
| MOTA | 4150 | OD1 ASN | IB 145 | 43.804 | | 82.472 | 1.00 22.69 |
| ATOM | 4151 | ND2 ASN | IB 145 | 43.693 | -5.819 | | |
| | 4152 | C ASI | N B 145 | 41.780 | -3.918 | 78.955 | 1.00 21.18 |
| MOTA | | | V B 145 | 41.389 | -5.002 | 78.508 | 1.00 17.80 |
| ATOM | 4153 | | | 42.293 | -2.968 | 78.177 | 1.00 15.23 |
| MOTA | 4154 | | 1 B 146 | | -3.175 | 76.733 | 1.00 19.71 |
| ATOM | 4155 | CA ASI | N B 146 | 42.367 | | | 1.00 17.65 |
| ATOM | 4156 | CB ASI | N B 146 | 42.773 | -1.880 | 76.015 | 1.00 19.86 |
| | 4157 | | N B 146 | 44.196 | -1.458 | 76.306 | |
| MOTA | | 001 361 | N B 146 | 45.109 | -1.735 | 75.532 | 1.00 20.27 |
| MOTA | 4158 | ODI ASI | N D 146 | 44.395 | -0.798 | 77.435 | 1.00 11.85 |
| ATOM | 4159 | ND2 ASI | N B 146 | | -4.342 | 76.331 | 1.00 19.07 |
| MOTA | 4160 | | N B 146 | 43.277 | | 75.328 | 1.00 18.61 |
| . ATOM | 4161 | O ASI | N B 146 | 43.030 | -4.996 | | 1.00 17.78 |
| | 4162 | N PRO | о в 147 | 44.358 | -4.598 | 77.082 | |
| MOTA | | | В 147 | 44.953 | -3.919 | 78.240 | 1.00 18.13 |
| ATOM | 4163 | | | 45.197 | -5.735 | 76.678 | 1.00 19.98 |
| ATOM | 4164 | | о в 147 | | | 77.698 | 1.00 24.29 |
| MOTA | 4165 | | D B 147 | 46.338 | -5.694 | | 1.00 26.27 |
| ATOM | 4166 | CG PR | ов 147 | 46.425 | -4.201 | 78.020 | 1.00 20.27 |
| ATOM | | C DE | о в 147 | 44.377 | -7.041 | 76.757 | 1.00 20.91 |
| MOTA | 4167 | C PRO | D D 147 | 44.461 | -7.892 | 75.871 | 1.00 17.58 |
| MOTA | 4168 | O PR | о в 147 | | -7.172 | .77.809 | |
| ATOM | 4169 | N AL | A B 148 | 43.568 | | 78.008 | |
| ATOM | 4170 | CA AL | A B 148 | 42.732 | -8.362 | | |
| | | CB AL | A B 148 | 42.049 | -8.312 | 79.372 | |
| ATOM | 4171 | C 31 | A B 148 | 41.683 | -8.473 | 76.903 | 1.00 22.58 |
| ATOM | 4172 | C AL | 3 5 140 | 41.419 | -9.567 | 76.404 | 1.00 18.38 |
| ATOM | 4173 | O AL | A B 148 | | | | |
| ATOM | 4174 | N VA | L B 149 | 41.080 | -7.341 | | |
| | 4175 | CA VA | L B 149 | 40.086 | -7.300 | | 1.00 10.04 |
| ATOM | | | L B 149 | 39.503 | -5.8 77 | 75.281 | 1.00 18.96 |
| ATOM | 4176 | | L B 149 | 38.691 | -5.800 | 73.988 | 1.00 17.32 |
| MOTA | 4177 | | 7 D 14C | 38.621 | -5.531 | | 1.00 15.33 |
| ATOM | 4178 | CG2 VA | L B 149 | 30.021 | | | |
| | 4179 | c va | ь в 149 | 40.763 | -7.709 | | |
| ATOM | 4180 | o va | L B 149 | 40.240 | -8.535 | 77 000 | 1.00 21.00 |
| ATOM | 1101 | | у в 150 | 41.927 | -7.120 | 73.903 | 1.00 19.51 |
| ATOM | 4181 | N GL | | 4.4 : | | | |
| | | | | | | | |

| MOTA | 4182 | . CA | GLY B 150 |) | 42.657 | -7.433 | 72.689 | 1.00 | 19.32 |
|-------|---------------|------|-------------|---|--------|----------|--------|------|----------------|
| MOTA | 4183 | C | GLY B 150 |) | 43.033 | | 72.606 | | 19.59 |
| ATOM | 4184 | 0 | GLY B 150 |) | 42.862 | | 71.568 | | 22.28 |
| MOTA | 4185 | N | ILE B 151 | | 43.558 | | 73.700 | | 19.51 |
| ATOM | 4186 | | | | | -10.834 | 73.723 | | 23.21 |
| ATOM | 4187 | | | | | -11.175 | 75.053 | | 23.50 |
| ATOM | 4188 | | | | | -12.679 | 75.158 | | 20.01 |
| ATOM | 4189 | | - | | | -10.394 | 75.129 | | 21.98 |
| ATOM | 4190 | | | | | -10.502 | 76.457 | | |
| ATOM | 4191 | | ILE B 151 | | | -11.741 | 73.490 | | 21.24 |
| ATOM | 4192 | | ILE B 151 | | | -12.692 | 72.706 | | 28.40 |
| ATOM | 4193 | | GLU B 152 | | | -12.692 | | | 22.96 |
| MOTA | 4194 | | - | | | | 74.144 | | 27.32 |
| | 4195 | | | | | -12.265 | 73.939 | | 27.62 |
| MOTA | | | | | | -11.845 | 74.886 | | 26.46 |
| ATOM | 4196 | | GLU B 152 | | | -12.200 | 76.347 | | 28.26 |
| ATOM | 4197 | - | | | | -13.708 | 76.592 | | 31.10 |
| ATOM | 4198 | | 1 GLU B 152 | | | -14.123 | 77.767 | | 29.55 |
| ATOM | 4199 | OE: | | | | -14.481 | 75.617 | | 30.51 |
| ATOM | 4200 | C | GLU B 152 | • | | -12.125 | 72.497 | | 30.30 |
| ATOM | 4201 | 0 | GLU B 152 | | | -13.082 | 71.893 | | 25.58 |
| ATOM | 4202 | N | TYR B 153 | | | -10.923 | 71.948 | | 26.23 |
| ATOM | 4203 | CA | TYR B 153 | | | -10.669 | 70.563 | | 28.19 |
| ATOM | 4204 | CB | TYR B 153 | | 40.082 | -9.235 | 70.190 | | 27.94 |
| ATOM | 4205 | CG | TYR B 153 | | 39.879 | | 68.735 | | 28.46 |
| MOTA | 4206 | CD: | | | 38.618 | | 68.240 | 1.00 | 25.69 |
| ATOM | 4207 | CE: | | | 38.447 | -8.195 | 66.898 | | 30.73 |
| ATOM | 4208 | CD | | | 40.962 | -8.847 | 67,856 | | 24.82 |
| ATOM | 4209 | CE: | - | • | 40.801 | -8.488 | 66.526 | | 29.26 |
| ATOM | 4210 | CZ | TYR B 153 | | 39.547 | | 66.054 | | 31.25 |
| ATOM | 4211 | он | TYR B 153 | | 39.406 | -7.803 | 64.735 | | 34.22 |
| ATOM | 4212 | С | TYR- B 153 | | | -11.627 | 69.674 | | 28.11 |
| MOTA | 4213 | 0 | TYR B 153 | | | -12.248 | 68.759 | 1.00 | 22.06 |
| MOTA | 4214 | N | LEU B 154 | | | -11.725 | 69.944 | 1.00 | 26.77 |
| ATOM | 4215 | .CA | LEU B 154 | | 42.681 | -12.:597 | 69.168 | 1.00 | 28.79 |
| MOTA | 4216 | CB | LEU B 154 | | | -12.386 | 69.592 | 1.00 | 28.06 |
| ATOM | 4217 | CG | LEU B 154 | | | -11.087 | 69.083 | | 27.71 |
| MOTA | 4218 | CDI | | | | -10.860 | 69.759 | | 34.15 |
| MOTA | 4219 | CD2 | | | | -11.171 | 67.571 | | 26.71 |
| ATOM | 4220 | C | LEU B 154 | | | -14.074 | 69.274 | | 26.98 |
| MOTA | 4221 | 0 | LEU B 154 | | | -14.787 | 68.271 | | 29.88 |
| MOTA | 1222 | N | ARG B 155 | | | -14.536 | 70.480 | | 23.19 |
| MOTA | 4223 | CA | ARG B 155 | | | -15.936 | 70.669 | | 29.47 |
| ATOM | 4224 | CB | ARG B 155 | | | -16.230 | 72.144 | | 28.53 |
| ATOM | 4225 | CG | ARG B 155 | | | -15.965 | 73.053 | 1.00 | 35.03 |
| ATOM | 4226 | CD | ARG B 155 | | | -16.276 | 74.507 | 1.00 | 39.42 |
| ATOM | 4227 | ΝE | ARG B 155 | | | -17.706 | 74.792 | | 30.99 |
| ATOM | 4228 | CZ | ARG B 155 | | | -18.209 | 75.986 | | 41.33 |
| MOTA | 4229 | NH1 | | | 41.591 | -17.394 | 77.002 | 1.00 | 38.47 |
| MOTA | 4230 | NH2 | | | 41.872 | -19.523 | 76.178 | 1.00 | 40.67 |
| MOTA | 4231 | С | ARG B 155 | | | -16.260 | 69.832 | 1.00 | |
| ATOM | 4232 | 0 | ARG B 155 | | 40.325 | -17.311 | 69.203 | 1.00 | 25.31 |
| ATOM | 4233 | Ŋ | LYS B 156 | | | -15.357 | 69.828 | 1.00 | 28.99 |
| MOTA | 4234 | CA | LYS B 156 | | | -15.573 | 69.038 | 1.00 | 34.63 |
| ATOM | 4235 | CB | LYS B 156 | | 37.148 | -14.534 | 69.386 | 1.00 | 3 6 .63 |
| ATOM | 4236 | CG | LYS B 156 | | 36.393 | -14.883 | 70.646 | 1.00 | 42.18 |
| ATCM | 4237 | CD | LYS B 156 | | | -14.900 | 71.868 | | 51.38 |
| ATOM | 423 ,8 | CE | LYS B 156 | | 36.685 | -15.712 | 73.009 | | 52.76 |
| ATOM | 4239 | NZ | LYS B 156 | | 36.561 | -17.172 | 72.677 | | 51.29 |
| ATOM. | 4240 | С | LYS B 156 | | 38.504 | -15.562 | 67.538 | | 34.66 |
| ATOM | 4241 | 0 | LYS B 156 | | 37.722 | -16.088 | 66.754 | | 33.53 |
| ATCM | 4242 | N | LYS B 157 | | | -14.966 | 67.140 | 1.00 | 30.06 |
| ATOM | -243 | CA | LYS B 157 | | | -14.945 | 65.734 | | 31.36 |
| ATCM | 1244 | CB | LYS B 157 | | | -13.746 | 65.418 | | 29.79 |
| ATOM | 4245 | CG | LYS B 157 | | | -12.426 | 65.359 | 1.00 | 31.52 |
| ATOM | 4246 | CD | LYS B 157 | | | -12.424 | 64.239 | 1.00 | 28.48 |
| ATCM | 4247 | CE | LYS B 157 | | | -11.101 | 64.171 | 1.00 | 31.90 |
| | | | | | | | | | |

PCT/US00/24700

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```
37.406 -11.080
                                                    63.054
                                                             1.00 32.91
                  LYS B 157
        4248
              NZ
ATOM
                                                              1.00 31.92
                                                    65.381
                  LYS B 157
                                   40.724 -16.234
        4249
              C
MOTA
                                   41.146 -16.421
                                                    64.246
                                                              1.00 33.58
                   LYS B 157
        4250
ATOM
                                                    66.368
                                                              1.00 28.97
        4251
                  GLY B 158
                                   40.890 -17.111
              N
MOTA
                                   41.546 -18.379
                                                    66.112
                                                              1.00 28.98
                  GLY B 158
        4252
              CA
ATOM
                                   42.962 -18.569
                                                    66.622
                                                              1.00
                                                                   33.33
                   GLY B 158
        4253
              C
MOTA
                                                    66.522
                                                              1.00 30.58
                                   43.503 -19.672
        4254
              O
                  GLY B 158
ATOM
                                                              1.00 32.80
                                                    67.164
                  PHE B 159
                                   43.578 -17.521
        4255
ATOM
              N
                                                    67.678
                                                              1.00 28.89
        4256
                  PHE B. 159
                                   44.937 -17.657
              CA
ATOM
                                                              1.00 30.33
                                                    67.934
                                   45.560 -16.286
                  PHE B 159
        4257
              CB -
ATOM
                                   45.748 -15.470
                                                     66.692
                                                              1.00 28:53
                  PHE B 159
        4258
              CG
ATOM
                                                     66.121
                                                              1.00 24.58
                                   44.682 -14.787
                  PHE B 159
              CD1
        4259
ATOM
                                                              1.00 24.21
                                                     66.068
                                   46.989 -15.420
                  PHE B 159
        4260
              CD2
ATOM
                                                              1.00 25.26
                                   44.849 -14.066
                                                     64.948
                  PHE B 159
        4261
              CE1
ATOM
                                                     64.895
                                                              1.00 23.66
                                   47.168 -14.706
                  PHE B 159
        4262
              CE2
ATOM
                                                              1.00 26.65
                                   46.095 -14.026
                                                     64.332
                  PHE B 159
        4263
              cz
ATOM
                                   44.969 -18.484
                                                     68.958
                                                              1.00 30.92
                   PHE B 159
        4264
ATOM
                                                     69.820
                                                              1.00 24.26
                                   44.102 -18.334
                   PHE B 159
              0
        4265
ATOM
                                                              1.00 28.86
                                                     69.077
                   LYS B 160
                                   45.979 -19.347
        4266
              N
ATOM
                                   46.123 -20.224
                                                     70.237
                                                              1.00 30.27
                  LYS B 160
              CA
ATOM
        4267
                                   46.085 -21.692
                                                              1.00 32.05
                                                     69.800
                  LYS B 160
        4268
              CB
MOTA
                                                              1.00 41.13
                                                     69.113
                   LYS B 160
                                   44.806 -22.117
        4269
              CG
MOTA
                                                              1.00 40.73
                                   44.809 -23.621
                                                     68.826
                  LYS B 160
        4270
              CD
ATOM
                                   45.945 -24.031
                                                     67.904
                                                              1.00 43.16
                  LYS B 160
        4271
              CE
ATOM
                                                     66:554
                                                              1.00 48.69
        4272
              NZ
                  LYS B 160
                                   45.812 ~23.408
ATOM
                                                              1.00 28.23
                                                     71.048
                   LYS B 160
                                   47.394 -19.997
        4273
              Ç
ATOM
                                                     72.130
                                                              1.00 25.29
                                   47.552 -20.561
                  LYS B 160
        4274
MOTA
                                   48.320 -19.206
                                                              1.00 28.51
                                                     70.520
        4275
              N
                   ARG B 161
ATOM
                                                              1.00 25.84
                                                     71.247
                   ARG B 161
                                    49.550 -18.921
              CA
        4276
ATOM
                                   50.724 -19.719
50.551 -21.245
                                                     70.667
                                                              1.00 25.33
                   ARG B 161
        4277
              CB
ATOM
                                                     70.781
                                                              1.00 27.47
        4278
              CG
                   ARG B 161
MOTA
                                                     70.394
                                                              1.00 32.27
                                   51.833 -21.985
        4279
                   ARG B 161
              CD
MOTA
                                                              1.00 34.90
                                   52.218 -21.761
                                                     69.002
                   ARG B 161
ATOM
        4280
              NE
                                   51.584 -22.276
                                                              1.00 38.45
                                                     67.954
        4281
              CZ
                   ARG B 161
MOTA
                                    50.527 -23.056
                                                     68.130
                                                              1.00
                                                                    38.77
                  ARG B 161
              NH1
        4282
 ATOM
                                                     66.725
                                                              1.00 38.64
                                    51.999 -22.000
                  ARG B 161
              NH2
ATOM
        4283
                                                     71.182
                                                              1.00 30.40
                                    49.818 -17.421
MOTA
        4284
              C
                   ARG B 161
                                    50.393 -16.912
                                                              1.00 27.50
                                                     70.218
                   ARG B 161
        4285
 ATOM
                                                               1.00 25.64
                                                     72.221
                                    49.376 -16.722
                   ILE B 162
atom
        4286
              N
                                                     72.303
                                                               1.00 27.44
                                    49.515 -15.273
                   ILE B 162
        4287
              CA
 MOTA
                                                               1.00 24.53
                                                     72.545
                                    48.134 -14.618
        4288
              CB
                   ILE B 162
 MOTA
                                    48.249 -13.101
                                                     72.473
                                                               1.00 25.49
        4289
                   ILE B 162
              CG2
 ATOM
                                                     71.487
                                                               1.00 29.46
                                    47.142 -15.101
                   ILE B 162
        4290
              CG1
 ROTA
                                   .45.688 -14.707
50.465 -14.868
                                                               1.00 31.94
                                                     71.758
        4291
                  ILE B 162
              CD1
 ATOM
                                                     73.429
                                                               1.00 22.68
                   ILE B 162
        4292
              C
 ATOM
                                                     74.568
                                                               1.00 24.25
                                    5^.311 -15.302
                   ILE B 162
        4293
              0
 ATOM
                                                               1.00 19.49
                                    5 _ . 454 - 14 . 042
                                                     73.100
                   LEU B 163
        4294
              N
 ATOM
                                                               1.00 17.57
                                    51.425 -13.561
                                                     74.081
        4295
                   LEU B 163
              CA
 ATOM
                                                               1.00 20.54
                                    53.850 -13.686
                                                      73.528
                   LEU B 163
 ATOM
        4296
              CB
                                                               1.00 18.84
                                                     74.295
                                    54.979 -12.975
                   LEU B 163
        4297
              CG
 TOM
                                                               1.00 20.55
                                    55.102 -13.538
                                                     75.690
                   LEU B 163
        4298
              CD1
 ATOM
                                                               1.00 18.57
                                                     73.556
                                    56.293 -13.148
                  LEU B 163
        4299
              CD2
 ATOM
                                                     74.430
                                                               1.00 16.20
                                    52.158 -12.099
                   LEU B 163
        4300
              С
 ATCM
                                                               1.00.16.09
                                    51.898 -11.277
                                                      73.549
                   LEU B 163
        4301
              О
 MOTA
                                                               1.00 14.05
                                    52.227 -11.780
                                                      75.715
                   TYR B 164
        4302
              N
 ATOM
                                                               1.00 16.21
                                                      76.191
                                    52.027 -10.411
                   TYR B 164
        4303
              CA
 ROTE
                                                               1.00 16.01
                                    50.777 -10.323
                                                      77.070
                   TYR B 164
        4304
              СЗ
 ATOM
                                                      77.667
                                                               1.00 15.08
                                            -8.948
                                    50.534
        4305
              CG
                   TYR B 164
 ATOM
                                                               1.00 19.51
                                                      76.869
                                    50.148
                                             -7.869
                  TYR B 164
        4306
              CD1
 ROTE
                                                               1.00 12.88
                                    49.948
                                             -6.597
                                                      77.418
                   TYR 5 164
        4307
              CE1
 ATOM
                                             -8.724
                                                      79.021
                                                               1.00 14.07
                                    50.715
                   TYR B 164
        4308
              CD2
 ATOM
                                                      79.583
                                                               1.00 13.66
                                    50.520
                                             -7.463
                   TYR B 164
        4309
              CE2
 RICH
                                                               1.00 14.72
                                    50.139
                                             -6.407
                                                      78.782
                   TYR B 164
        4310
              cz
 ATOM
                                                               1.00 13.54
                                                      79.354
                                    49.952
                                            -5.163
                   TYR B .164
              OH
 ATOM
        4311
                                                      77.018
                                                               1.00 19.14
                   TYR B 164
                                    53.246 -10.017
        4312
              С
                                                               1.00 26.51
 -TOM
                                                    78.036
                                    53.539 -10.642
                   TYR B 164
              0
        4313
 ATOM
```

| MOTA | 4314 | N | ILE : | 3 165 | 53.964 | -8.992 | 76.573 | 1.00 22.40 |
|-------|------|-----|--------|-------|----------|--------|----------------|------------|
| | 4315 | CA | TI.E 1 | 3 165 | 55.148 | -8.518 | 77.285 | 1.00 17.72 |
| MOTA | | | | | | | | |
| MOTA | 4316 | CB | ILE 1 | 3 165 | 56.352 | -8.465 | 76.343 | 1.00 22.51 |
| | 4317 | CG2 | ILE 1 | 3 165 | 57.582 | -7.902 | 77.079 | 1.00 16.36 |
| ATOM | | | | | | | | • |
| MOTA | 4318 | CG1 | ILE ! | 3 165 | 56.632 | -9.880 | 75.818 | 1.00 19.82 |
| | 4319 | CDl | TLE 1 | 3 165 | 57.721 | -9.942 | 74.742 | 1.00 21.74 |
| ATOM | | | | | | | | |
| ATOM | 4320 | С | ILE | 3 165 | 54.851 | -7.126 | 77.850 | 1.00 22.54 |
| MOTA | 4321 | 0 | TUE | 3 165 | 54.478 | -6.223 | 77.111 | 1.00 16.60 |
| | | | | | | | | 1.00 15.78 |
| ATOM | 4322 | N | ASP I | 3 166 | 55.046 | -6.961 | 79.156 | |
| ATOM | 4323 | CA | ASP I | 3 166 | 54.740 | -5.704 | 79.840 | 1.00 20.62 |
| | | | | | | -5.996 | 80.949 | 1.00 17.57 |
| ATOM | 4324 | CB | ASP I | | | | | |
| MOTA | 4325 | CG | ASP I | 3 166 | 53.063 | -4.742 | 81.486 | 1.00 25.39 |
| | | OD1 | | | 53.779 | -3.859 | 82.003 | 1.00 19.68 |
| MOTA | 4326 | | | | | | | |
| MOTA | 4327 | OD2 | ASP I | 3 166 | 51.824 | -4.637 | 81.377 | 1.00 29.22 |
| ATOM | 4328 | Ċ | ASP I | 166 | 55.976 | -5.002 | 80.423 | 1.00 19.01 |
| | | | | | | -5.412 | 81.456 | 1.00 19.74 |
| MOTA | 4329 | 0 | ASP I | 2 TOO | 56.509 | _ | | |
| ATOM | 4330 | N | LEU I | 3 167 | 56.414 | -3.923 | 79.775 | 1.00 17.88 |
| | | CA | LEU I | | 57.598 | -3.211 | 80.235 | 1.00 14.99 |
| MOTA | 4331 | | | | | | | |
| MOTA | 4332 | CB | LEU I | 3 167 | 58.412 | -2.710 | 79.044 | 1.00 19.22 |
| MOTA | 4333 | CG | LEU I | 3 167 | 58.871 | -3.799 | 78.069 | 1.00 22.68 |
| | | | | | | -3.179 | 77.074 | 1.00 25.35 |
| MOTA | 4334 | | LEU I | | 59.835 | | | |
| MOTA | 4335 | CD2 | LEU I | 3 167 | 59.570 | -4.943 | 78.808 | 1.00 17.54 |
| | 4336 | С | LEU I | 3 167 | 57.284 | -2.059 | 81.183 | 1.00 17.49 |
| ATOM | | | | | | | | |
| ATOM | 4337 | 0 | LEU I | 3 167 | 58.189 | -1.359 | 81.639 | |
| MOTA | 4338 | N | ASP I | 168 | 56.003 | -1.878 | 81.479 | 1.00 20.03 |
| | | | | | 55.549 | -0.848 | 82.412 | 1.00 21.98 |
| MOTA | 4339 | CA | ASP I | | | | | |
| MOTA | 4340 | CB | ASP I | 3 168 | 54.030 | -0.955 | 82.59 7 | 1.00 21.21 |
| | 4341 | CG | ASP I | 168 | 53.453 | 0.186 | 83.428 | 1.00 24.92 |
| MOTA | | | | | | | 83.753 | 1.00 22.98 |
| MOTA | 4342 | С | ASP E | 168 | 56.241 | -1.139 | | |
| MOTA | 4343 | 0 | ASP I | 168 | 56.447 | -2.304 | 84.091 | 1.00 18.36 |
| | 4344 | | ASP I | | 52.849 | 1.099 | 82.825 | 1.00 22.03 |
| MOTA | | | | | | | 84.676 | 1.00 18.43 |
| MOTA | 4345 | OD2 | ASP E | 168 | 53.606 | 0.189 | | |
| MOTA | 4346 | N | ALA I | 169 | 56.581 | -0.095 | 84.514 | 1.00 15.46 |
| | 4347 | CA | ALA E | 169 | . 57.263 | -0.268 | 85.807 | 1.00 18.73 |
| MOTA | | | | | 57.764 | 1.084 | 86.323 | 1.00 11.98 |
| ATOM | 4348 | CB | ALA I | | | | | • |
| MOTA | 4349 | С | ALA E | 169 | 56.400 | -0.940 | 86.886 | 1.00 21.82 |
| ATOM | 4350 | 0 | ALA E | 169 | 56.886 | -1.262 | 87.980 | 1.00 22.51 |
| | | | HIS E | | 55.120 | -1.134 | 86.600 | 1.00 18.75 |
| ATOM | 4351 | N | | | | | 87.570 | 1.00 22.70 |
| ATOM | 4352 | CA | HIS E | 170 | 54.238 | -1.776 | | |
| MOTA | 4353 | С | HIS E | 170 | 53.716 | -3.096 | 87.015 | 1.00 22.11 |
| | 4354 | o | HIS E | | 53.536 | -3.244 | 85.809 | 1.00 21.94 |
| MOTA | | | | | | -0.867 | 87.927 | 1.00 21.28 |
| MOTA | 4355 | CB | HIS E | | 53.050 | | | |
| ATOM | 4356 | CG | HIS E | 170 | 53.449 | 0.475 | 88.460 | 1.00 18.89 |
| | 4357 | ND1 | HIS E | 170 | 53.695 | 1.539 | 87.626 | 1.00 19.13 |
| MOTA | | | | | | 2.539 | 88.412 | 1.00 19.41 |
| ATOM | 4358 | | HIS E | | 54.046 | | | |
| MOTA | 4359 | CD2 | HIS E | 170 | 53.660 | 0.854 | 89.746 | 1.00 19.02 |
| MOTA | 4360 | NE2 | HIS E | 170 | 54.042 | 2.174 | 89.710 | 1.00 20.45 |
| | | | | | 53.474 | -4.047 | 87.907 | 1.00 19.20 |
| ATOM | 4361 | N | HIS E | | | | | 1.00 21.20 |
| ATOM | 4362 | CA | HIS E | 171 | 52.961 | -5.352 | 87.519 | |
| | 4363 | CB | HIS E | 171 | 52.964 | -6.284 | 88.722 | 1.00 22.00 |
| MOTA | | | | | | -7.683 | 88.400 | 1.00 24.64 |
| MOTA | 4364 | CG | HIS E | | 52.541 | | | |
| MOTA | 4365 | CD2 | HIS E | 171 | 53.056 | -8.594 | 87.540 | 1.00 19.19 |
| | 4366 | | HIS E | | 51.441 | -8.279 | 88.979 | 1.00 25.71 |
| MOTA | | | | | 51.295 | -9.497 | 88.487 | 1.00 25.30 |
| MOTA | 4367 | | HIS E | | | | | |
| ATOM | 4368 | NE2 | HIS E | 171 | 52.261 | -9.713 | 87.612 | 1.00 24.71 |
| ATOM. | 4369 | С | HIS E | 171 | 51.549 | -5.306 | 86.943 | 1.00 23.91 |
| | | | | | | -4.620 | 87.479 | 1:00 18.93 |
| ATOM | 4570 | 0 | HIS E | | 50.677 | | | |
| ATOM | 4371 | N | CYS. E | 172 | 51.332 | -6.062 | 85.865 | 1.00 15.36 |
| ATOM | 4372 | CA | CYS 3 | | 50.036 | -6.141 | 85.207 | 1.00 20.03 |
| | | | | | | -6.534 | 83.732 | 1.00 22.46 |
| ATOM | 4373 | CB | CYS E | | 50.240 | | | 1.00 22 40 |
| ATOM | 4374 | 5G | CYS E | 172 | 51.259 | -3.030 | 83.419 | 1:00 23.49 |
| ATOM | 4375 | С | CYS E | 172 | 49.110 | -7.146 | 85.913 | 1.00 18.05 |
| | | | CYS E | | 48.712 | -8.151 | 85.327 | 1.00 18.23 |
| atom | 4376 | 0 | | 177 | 48.767 | | 87.170 | 1.00 16.78 |
| ATOM | 4377 | N | ASP E | 1/3 | | -6.871 | | |
| MOTA | 4378 | CA | ASP E | 173 | 47.909 | -7.776 | 87.928 | 1.00 18.81 |
| | 1379 | СВ | ASP E | 173. | 47.638 | -7.236 | 89.344 | 1.00 20.39 |
| ATCM | 30.0 | | | | | | • | |

| ATOM | 4380 | CG | ASP | В | 173 | 46.961 | -5.871 | 89.354 | 1.00 23.40 |
|------|------|-----|-----|----|-----|--------|----------|--------|------------|
| ATOM | 4381 | OD1 | ASP | В | 173 | 46.564 | ~5.435 | 90.455 | 1.00 18.64 |
| | 4382 | | ASP | | 173 | 46.834 | -5.231 | 88.291 | 1.00 19.24 |
| MOTA | | C | ASP | | | 46.595 | -8.116 | 87.219 | 1.00 17.46 |
| MOTA | 4383 | | ASP | | | 46.162 | -9.272 | 87.224 | 1.00 15.53 |
| ATOM | 4384 | 0 | | | | | | 86.580 | 1.00 13.46 |
| ATOM | 4385 | N | GLY | | | 45.978 | -7.130 | | 1.00 18.18 |
| ATOM | 4386 | CA | GLY | | 174 | 44.733 | -7.391 | 85.876 | |
| ATOM | 4387 | С | GLY | В | 174 | 44.904 | -8.392 | 84.741 | 1.00 17.85 |
| MOTA | 4388 | 0 | GLY | В | 174 | 44.104 | -9.316 | 84.583 | 1.00 18.27 |
| ATOM | 4389 | N | VAL | В | 175 | 45.951 | -8.214 | 83.943 | 1.00 16.14 |
| | 4390 | CA | VAL | | 175 | 46.206 | -9.111 | 82.829 | 1.00 17.00 |
| MOTA | | CB | VAL | | 175 | 47.305 | -8.552 | 81.902 | 1.00 27.22 |
| ATOM | 4391 | | VAL | | | 47.533 | -9.507 | 80.731 | 1.00 19.75 |
| MOTA | 4392 | CGI | VAL | Φ. | 175 | 46.896 | -7.169 | 81.396 | 1.00 18.66 |
| MOTA | 4393 | | VAL | | | | | 83.324 | 1.00 22.82 |
| ATOM | 4394 | С | VAL | | | | -10.486 | | 1.00 18.06 |
| MOTA | 4395 | o | VAL | | | | -11.503 | 82.754 | |
| MOTA | 4396 | N | | | 176 | | -10.520 | 84.378 | 1.00 21.67 |
| ATOM | 4397 | CA | GLN | В | 176 | 47.889 | -11.798 | 84.911 | 1.00 21.55 |
| ATOM | 4398 | CB | GLN | В | 176 | 48.824 | -11.602 | 86.105 | 1.00 19.68 |
| ATOM | 4399 | CG | GLN | В | 176 | 49.088 | -12.905 | 86.862 | 1.00 20.17 |
| | 4400 | CD | GLN | | 176 | 50.066 | -12.759 | 87.996 | 1.00 25.42 |
| MOTA | 4401 | | GLN | | 176 | | -12.442 | 87.786 | 1.00 21.56 |
| ATOM | | NE2 | | | | | -13.000 | 89.217 | 1.00 20.18 |
| ATOM | 4402 | | | | | | -12.630 | 85.348 | 1.00 24.78 |
| MOTA | 4403 | С | GLN | | 176 | | -13.817 | 85.057 | 1.00 22.91 |
| MOTA | 4404 | 0 | GLN | | 176 | | | 86.051 | 1.00 23.69 |
| MOTA | 4405 | N | GLU | | 177 | | -12.007 | | |
| ATOM | 4406 | CA | GLU | | 177 | | -12.727 | 86.523 | 1.00 27.01 |
| ATOM | 4407 | CB | GLU | В | 177 | | -11.825 | 87.394 | 1.00 24.73 |
| ATOM | 4408 | CG | GLU | В | 177 | 42.633 | -12.581 | 88.138 | 1.00 37.46 |
| ATOM | 4409 | CD | GLU | В | 177 | 41.767 | -11.676 | 88.987 | 1.00 42.48 |
| ATOM | 4410 | OE1 | | | 177 | 40.875 | -11.002 | 88.432 | 1.00 44.35 |
| | 4411 | | GLU | | 177 | | -11.627 | 90.213 | 1.00 45.63 |
| MOTA | | C | GLU | | 177 | | -13.247. | 85.370 | 1.00 26.56 |
| MOTA | 4412 | | GLU | | | | -14.375 | 85.408 | 1.00 27.71 |
| MOTA | 4413 | 0 | | | 178 | | -12.418 | 84.344 | 1.00 24.58 |
| ATOM | 4414 | N | ALA | | | | -12.775 | 83.174 | 1.00 25.86 |
| MOTA | 4415 | CA | ALA | | 178 | | | 82.171 | 1.00 24.20 |
| MOTA | 4416 | CB | ALA | | 178 | | -11.628 | 82.485 | 1.00 25.72 |
| ATOM | 4417 | С | ALA | | 178 | | -14.054 | _ | 1.00 22.38 |
| MOTA | 4418 | 0 | ALA | | 178 | | -14.838 | 82.036 | 1.00 27.19 |
| MOTA | 4419 | N | PHE | | 179 | | -14.282 | 82.395 | |
| ATOM | 4420 | CA | PHE | В | 179 | | -15.489 | 81.703 | 1.00 27.05 |
| ATOM | 4421 | CB | PHE | В | 179 | 45.714 | -15.086 | 80.418 | 1.00 25.22 |
| ATOM | 4422 | CG | PHE | В | 179 | 44.992 | -14.020 | 79.644 | 1.00 20.36 |
| ATOM | 4423 | | PHE | В | 179 | 45.387 | -12.687 | 79.735 | 1.00 25.23 |
| - | 4424 | | PHE | | 179 | 43.860 | -14.332 | 78.902 | 1.00 19.22 |
| ATOM | 1425 | | PHE | | | | -11.677 | 79.102 | 1.00 19.25 |
| ATOM | | | PHE | | 179 | | -13.315 | 78.272 | 1.00 20.65 |
| MOTA | 4426 | CE2 | | | | | -12.0C1 | 78.374 | 1.00 25.64 |
| MOTA | 4427 | cz | PHE | | 179 | | -16.398 | 82.556 | 1.00 23.50 |
| ATOM | 4428 | С | PHE | | 179 | | | 82.038 | 1.00 18.26 |
| ATOM | 4429 | 0 | PHE | | | | -17.182 | 83.868 | 1.00 23.24 |
| MOTA | 4430 | N | TYR | | | | -16.313 | | 1.00 26.76 |
| MOTA | 4431 | CA | TYR | В | 180 | 46.479 | -17.106 | 84.799 | |
| ATOM | 4432 | CB | TYR | В | 180 | 46.150 | -16.665 | 86.231 | 1.00 25.72 |
| MOTA | 4433 | CG | TYR | В | 180 | 47.226 | -16.969 | 87.247 | 1.00 29.66 |
| | 4434 | | TYR | | | 47.037 | -17.942 | 88.237 | 1.00 27.07 |
| ATOM | 4435 | CE1 | | | | 48.039 | -18.222 | 89.170 | 1.00 30.08 |
| ATOM | 4436 | CD2 | TYR | | | 48.444 | -16.283 | 87.216 | 1.00 29.68 |
| ATOM | | | TYR | - | | 49 451 | -16.552 | 88.139 | 1.00 30.99 |
| ATCM | 4437 | | TYR | | | 40 240 | -17.521 | 89.112 | 1.00 33.16 |
| MOTA | 4438 | CZ | | | | 50 202 | -17.791 | 90.006 | 1.00 28.47 |
| ATOM | 1439 | OH | TYR | | | 16.202 | -10 610 | 84.649 | 1.00 29.13 |
| ATOM | 4440 | С | TYR | | | 40.200 | -18.619 | 84.922 | 1.00 23.43 |
| ATOM | 1441 | 0 | TYR | | | 4/.163 | -19.416 | | 1.00 25.67 |
| ATOM | 4442 | N | ASP | | | 45.073 | -19.021 | 84.190 | |
| ATOM | 4443 | CA | ASP | В | 181 | 44.784 | -20.445 | 84.075 | 1.00 28.28 |
| ATOM | 1144 | CB | ASP | | | 43.446 | -20.759 | 84.757 | 1.00 32.13 |
| ATCM | 1445 | CG | ASP | | | 42.247 | -20.410 | 83.890 | 1.00 36.12 |
| | | _ | | | | | | | |

| | | | * |
|-------|--------------------|-----------------|--|
| ATOM | 4446 OD1 ASP B 181 | 42.202 -19.30 | 0 83.329 1.00 41.04 |
| ATOM | 4447 OD2 ASP B 181 | 41.334 -21.24 | 9 83.782 1.00 44.36 |
| MOTA | 4448 C ASP B 181 | 44.773 -21.01 | 8 82.664 1.00 32.41 |
| MOTA | | 44.246 -22.11 | 5 82.444 1.00 31.67 |
| ATOM | | 45.345 -20.30 | 2 81.702 1.00 29.24 |
| MOTA | 4451 CA THR B 182 | 45.363 -20.823 | |
| MOTA | 4452 CB THR B 182 | 44.468 -20.00 | |
| ATOM | 4453 OG1 THR B 182 | 44.516 -20.59 | |
| MOTA | 4454 CG2 THR B 182 | 44.947 -18.56 | |
| ATOM | 4455 C THR B 182 | 46.759 -20.870 | |
| ATOM | 4456 O THR B 182 | - 47.591 -20.00 | |
| MOTA | 4457 N ASP B 183 | 46.999 -21.878 | |
| ATOM | 4458 CA ASP B 183 | 48.296 -22.049 | |
| ATÖM | 4459 CB ASP B 183 | 48.648 -23.536 | |
| MOTA | 4460 CG ASP B 183 | 47.718 -24.319 | |
| ATOM | 4461 OD1 ASP B 183 | 46.513 -23.988 | |
| MOTA | 4462 OD2 ASP B 183 | 48.186 -25.271 | |
| MOTA | 4463 C ASP B 183 | 48.321 -21.462 | |
| ATOM | 4464 O ASP B 183 | 49.332 -21.557 | |
| ATOM | 4465 N GLN B 184 | 47.217 -20.852 | |
| ATOM | 4466 CA GLN B 184 | 47.151 -20.251 | |
| ATOM | 4467 CB GLN B 184 | 45.712 -20.256 | |
| ATOM | 4468 CG GLN B 184 | 45.060 -21.632 | |
| ATOM | 4469 CD GLN B 184 | 43.760 -21.647 | |
| ATOM | 4470 OE1 GLN B 184 | 42.897 -20.789 | |
| ATOM | 4471 NE2 GLN B 184 | 43.611 -22.641 | 73.912 1.00 35.43 |
| ATOM | 4472 C GLN B 184 | 47.672 -18.817 | 72.870 1.00 28.92 75.175 1.00 27.28 |
| ATOM | 4473 O GLN B 184 | 47.871 -18.171 | |
| ATOM | 4474 N VAL B 185 | 47.900 -18.325 | |
| ATOM | 4475 CA VAL B 185 | 48.400 -16.972 | |
| ATOM | 4476 CB VAL B 185 | 47.304 -16.039 | 76.575 1.00 26.26 77.145 1.00 22.85 |
| ATOM | 4477 CG1 VAL B 185 | 47.879 -14.642 | |
| ATOM | 4478 CG2 VAL B 185 | 46.136 -15.967 | 77.395 1.00 23.10 76.191 1.00 21.67 |
| ATOM | 4479 C VAL B 185 | 49.570 -16.964 | 77.547 1.00 27.01 |
| MOTA | 4480 O VAL B 185 | 49.456 -17.469 | 78.663 1.00 23.75 |
| ATOM | 4481 N PHE B 186 | 50.696 -16.403 | 77.115 1.00 22.02 |
| ATOM | 4482 CA PHE B 186 | 51.868 -16.301 | 77.978 1.00 21.83 |
| ATOM | 4483 CB PHE B 186 | 53.142 -16.763 | 77.252 1.00 17.02 |
| ATOM | 4484 CG PHE B 186 | 54.336 -16.921 | 78.170 1.00 24.84 |
| ATOM | 4485 CD1 PHE B 186 | 54.756 -18.189 | 78.580 1.00 22.70 |
| ATOM | 4486 CD2 PHE B 186 | 55.004 -15.805 | 78.670 1.00 20.26 |
| ATOM | 4487 CE1 PHE B 186 | 55.819 -18.338 | 79.471 1.00 21.47 |
| ATOM | 4488 CE2 PHE B 186 | 56.071 -15.941 | 79.563 1.00 20.01 |
| MOTA | 4489 CZ PHE B 186 | 56.481 -17.206 | 79.968 1.00 17.84 |
| MOTA | 4490 C PHE B 186 | 52.032 -14.827 | 78.368 1.00 18.12 |
| YLO. | 4491 O PHE B 186 | 52.038 -13.946 | 77.508 1.00 15.92 |
| ATO.4 | 4492 N VAL B 187 | 52.161 -14.565 | 79.661 1.00 18.06 |
| ATOM | 4493 CA VAL B 187 | 52.348 -13.208 | 80.153 1.00 17.67 |
| ATOM | 4494 CB VAL B 187 | 51.282 -12.839 | 81.225 1.00 22.85 |
| MOTA | 4495 CG1 VAL B 187 | 51.608 -11.473 | 81.840 1.00 24.08 |
| ATOM | 4496 CG2 VAL B 187 | 49.882 -12.808 | 80.598 1.00 18.82 |
| MOTA | 4497 C VAL B 187 | 53.735 -13.060 | 80.788 1.00 18.32 |
| ATOM | 4498 O VAL B 187 | 54.092 -13.807 | 81.707 1.00 18.82 |
| MOTA | 4499 N LEU B 188 | 54.503 -12.103 | 80.282 1.00 14.70 |
| ATOM | 4500 CA LEU B 188 | 55.832 -11.789 | 80.798 1.00 18.84 |
| ATCM | 4501 CB LEU B 188 | 56.900 -11.948 | 79.716 1.00 18.64 |
| ATOM | 4502 CG LEU B 188 | 58.230 -11.277 | 80.082 1.00 21.23 |
| ATOM | 4503 CD1 LEU B 188 | 58.769 -11.832 | 81.395 1.00 18.55 |
| ATOM | 4504 CD2 LEU B 188 | 59.227 -11.489 | 78.957 1.00 20.49 |
| ATCM | 4505 C LEU B 188 | 55.836 -10.339 | 81.280 1.00 22.14 |
| ATOM | 4506 O LEU B 188 | 55.527 -9.410 | 80.517 1.00 19.96 |
| ATOM | 1507 N SER B 189 | 56.187 -10.133 | 82.540 1.00 21.08 |
| ATOM | 4508 CA SER B 189 | 56.203 -8.782 | 83.061 1.00 21.85 |
| ATOM | 4509 CB SER B 189 | 54.956 ~8.543 | 83.908 1.00 25.95 |
| ATCM | 4510 OG SER B 189 | 54.988 -7.252 | 84.475 1.00 21.91 |
| ATOM. | 4511 C SER B 189 | 57.423 -8.420 | 83.883 1.00 23.62 |

| * moM | 4512 | ο. | SER B | 189 | 57.829 | -9.174 | 84.766 | 1.00 18.61 |
|-------|-------|-----|-------|-------|--------|---------|--------|------------|
| ATOM | | | LEU B | 100 | 58.020 | -7.269. | 83.569 | 1.00 20.83 |
| MOTA | 4513 | N | | | 59.149 | -6.767 | 84.347 | 1.00 21.85 |
| MOTA | 4514 | CA | LEU B | | | | 83.473 | 1.00 22.85 |
| MOTA | 4515 | CB | | 190 | 60.278 | -6.226 | | 1.00 32.59 |
| ATOM | 4516 | CG | LEU B | 190 | 60.964 | -7.089 | 82.413 | |
| MOTA | 4517 | CD1 | LEU B | 190 | 62.337 | -6.479 | 82.140 | 1.00 29.27 |
| ATOM | 4518 | CD2 | LEU B | 190 | 61.136 | -8.511 | 82.879 | 1.00 31.88 |
| | 4519 | С | | 190 | 58.505 | -5.613 | 85.085 | 1.00 21.28 |
| MOTA | 4520 | ō | LEU B | | 57.695 | -4.897 | 84.501 | 1.00 15.72 |
| ATOM | 4521 | | | 191 | 58.857 | -5.421 | 86.351 | 1.00 18.16 |
| MOTA | | CA | | 191 | 58.249 | -4.357 | 87.145 | 1.00 17.46 |
| ATOM | 4522 | | | 191 | 56.759 | -4.690 | 87.369 | 1.00 16.00 |
| АТОМ | 4523 | CB | | 191 | 56.517 | -6.085 | 87.880 | 1.00 22.14 |
| ATOM | 4524 | CG | | | 56.341 | -6.551 | 89.143 | 1.00 12.25 |
| MOTA | 4525 | CD2 | HIS B | | 56.372 | -7.179 | 87.049 | 1.00 18.02 |
| MOTA | 4526 | ND1 | HIS B | | | -8.256 | 87.775 | 1.00 8.17 |
| ATOM | 4527 | | HIS B | 191 | 56.119 | | 89.049 | 1.00 19.79 |
| ATOM | 4528 | NE2 | HIS B | | 56.094 | -7.902 | | 1.00 17.41 |
| ATOM | 4529 | С | HIS B | | 58.945 | -4.197 | 88.484 | |
| MOTA | 4530 | 0 | | 191 | 59.769 | -5.029 | 88.867 | 1.00 18.74 |
| MOTA | 4531 | N | GLN B | 192 | 58.618 | -3.114 | 89.182 | 1.00 18.20 |
| | 4532 | CA | | 192 | 59.173 | -2.854 | 90.502 | 1.00 18.41 |
| MOTA | 4533 | CB | | 192 | 58.690 | -1.500 | 91.034 | 1.00 20.71 |
| ATOM | 4534 | CG | | 192 | 58.871 | -0.334 | 90.072 | 1.00 21.49 |
| ATOM | | CD | | 192 | 58.226 | 0.930 | 90.594 | 1.00 20.65 |
| ATOM | 4535 | | | 192 | 58.775 | 1.615 | 91.459 | 1.00 21.52 |
| MOTA | 4536 | OEl | | 192 | 57.029 | 1.226 | 90.098 | 1.00 15.10 |
| ATOM | 4537 | NE2 | | | 58.608 | -3.945 | 91.395 | 1.00 17.55 |
| MOTA | 4538 | С | _ | 192 | 57.415 | -4.256 | 91.320 | 1.00 17.48 |
| ATOM | 4539 | 0 | | 192 | | -4.522 | 92.240 | 1.00 15.71 |
| ATOM | 4540 | N | SER B | | 59.447 | -5.574 | 93.143 | 1.00 20.58 |
| ATOM | 4541 | CA | SER B | | 58.986 | | 94.120 | 1.00 20.71 |
| MOTA | 4542 | CB | SER B | | 60.093 | -5.963 | | 1.00 22.55 |
| MOTA | 4543 | OG | SER B | | 59.571 | -6.804 | 95.138 | 1.00 22.33 |
| ATOM | 4544 | С | SER B | 193 | 57.774 | -5.112 | 93.947 | - |
| ATOM | 4545 | 0 | SER B | | 57.769 | -4.003 | 94.486 | 1.00 20.82 |
| ATOM | 4546 | N | PRO B | 194 | 56.745 | -5.967 | 94.063 | 1.00 21.80 |
| ATOM | 4547 | CD | PRO B | | 56.648 | -7.331 | 93.524 | 1.00 24.27 |
| ATOM | 4548 | CA | PRO B | 194 | 55.524 | -5.643 | 94.812 | 1.00 23.58 |
| | 4549 | CB | PRO B | | 54.678 | -6.909 | 94.642 | 1.00 22.98 |
| MOTA | 4550 | CG | PRO B | | 55.168 | -7.458 | 93.317 | 1.00 26.35 |
| ATOM | 4551 | Č | PRO B | | 55.841 | -5.366 | 96.283 | 1.00 25.79 |
| MOTA. | 4552 | Ö | | 194 | 55.009 | -4.831 | 97.022 | 1.00 27.26 |
| ATOM | | N | GLU B | | 57.045 | -5.736 | 96.710 | 1.00 23.20 |
| ATOM | 4553 | | GLU B | 195 | 57.428 | -5.514 | 98.093 | 1.00 29.56 |
| atom | 4554 | CÀ | GLU B | | 58.816 | -6.090 | 98.379 | 1.00 32.38 |
| atom | 4555 | CB | | | 58.940 | -7.567 | | 1.00 45.25 |
| ATOM | 4556 | CG | | 195 | 60.206 | -8.189 | 98.613 | 1.00 50.44 |
| ATOM | 4557 | CD | GLU B | | _ | -7.580 | 98.471 | 1.00 50.51 |
| MOTA | 4558 | | GLU B | | 61.290 | -9.297 | 99.184 | .00 49.77 |
| MOTA | 4559 | OE2 | | 195 | 60.118 | | 98.425 | 1.00 25.11 |
| ATOM | 4560 | C | | 195 | 57.414 | -4.035 | 99.551 | 1.00 29.05 |
| ATOM | 4561 | 0 | GLU B | | 57.095 | ~3.659 | 97.445 | 1.00 22.90 |
| ATOM | 4562 | N | TYR B | 196 | 57.729 | -3.191 | | 1.00 22.46 |
| ATOM | 4563 | CA | TYR B | 196 - | 57.743 | -1.750 | 97.696 | 1.00 22.72 |
| ATCM | 4564 | CB | TYR B | 196 | 59.188 | -1.223 | 97.668 | 1.00 22.72 |
| ATOM | .4565 | CG | TYR B | 196 | 59.855 | -1.234 | 96.301 | 1.00 24.17 |
| | 4566 | | TYR B | 196 | 59.639 | -0.203 | 95.385 | 1.00 20.87 |
| ATOM | 4567 | CEI | | 196 | 60.229 | -0.222 | 94.118 | 1.00 18.31 |
| ATOM | 4568 | CD2 | | | 60.684 | -2.289 | 95.916 | 1.00 24.63 |
| MOTA | | CE2 | TYR B | | 61.276 | -2.318 | 94.648 | 1.00 24.39 |
| ATOM | 4569 | | TYR B | 196 | 61.042 | -1.284 | 93.756 | 1.00 23.01 |
| MOTA | 4570 | CZ | | | 61.592 | -1.328 | 92.492 | 1.00 19.86 |
| ATCM | 4571 | ОН | TYR B | 106 | 56.896 | -0.938 | 96.725 | 1.00 23.54 |
| ATOM | 4572 | C | TYR B | | | 0.275 | 96.869 | 1.00 17.53 |
| ATOM | 4573 | 0 | TYR B | 730 | 56.779 | -1.589 | 95.740 | 1.00 22.11 |
| ATOM | 4574 | N | ALA B | | 56.293 | | 94.779 | 1.00 24.28 |
| ATOM | 4575 | CA | ALA B | 197 | 55.503 | -0.829 | 93.513 | 1.00 23.03 |
| MOTA | 4576 | CB | ALA B | 197 | 56.310 | -0.616 | | 1.00 22.80 |
| ATOM | 1577 | С | ALA B | 197 | 54.153 | -1.412 | 94.413 | 1.00 22.00 |
| | | | | | | | | |

Figure 18-70

| ATOM | 4578 | O ALA B 197 | 53.91 | 0 -2.609 | 94.549 | 1.00 17.67 |
|--------------|----------------------|-------------------------------|------------------|----------------------|------------------|--------------------------|
| MOTA | | N PHE B 198 | 53.27 | | | |
| ATOM | | CA PHE B 198 | 51.95 | | | |
| ATOM | | CB PHE B 198 | 51.15 | 0.263 | 93.035 | |
| MOTA | | CG PHE B 198 | 49.72 | | | |
| ATOM | * | CD1 PHE B 198 | 48.73 | | | |
| ATOM | | CD2 PHE B 198 | 49.36 | | | 1.00 25.82 |
| MOTA | | CE1 PHE B 198 | 47.41 | | | |
| MOTA MOTA | | CE2 PHE B.198 CZ PHE B 198 | 48.05 | | | |
| MOTA | | CZ PHE B 198 C PHE B 198 | 47.07 | | | |
| ATOM | _ | O PHE B 198 | 52.17 53.04 | | | |
| MOTA | | N PRO B 199 | 51.40 | | | |
| ATOM | | CD PRO B 199 | 51.44 | 7 -2.952 0 -3.887 | | |
| MOTA | | CA PRO B 199 | 50.38 | | | |
| MOTA | 4593 | CB PRO B 199 | 49.54 | | | |
| MOTA | 4594 | G PRO B 199 | 50.64 | | | 1.00 35.88 |
| MOTA | | PRO B 199 | 51.24 | | | 1.00 36.93 |
| ATOM | 4596 | | 52.30 | | 93.860 | 1.00 50.93 |
| MOTA | 4597 N | | 50.80 | | 95.422 | 1.00 37.04 |
| MOTA | | A PHE B 200 | 51.64 | | 96.421 | 1.00 30.13 |
| ATOM | | B PHE B 200 | 51.54 | | 97.723 | 1.00 28.70 |
| MOTA MOTA | | G PHE B 200 | 51.76 | | 97.543 | 1.00 29.98 |
| ATOM | | D1 PHE B 200 D2 PHE B 200 | 50.71 | | 97.137 | 1.00 28.92 |
| MOTA | | E1 PHE B 200 | 53.010 50.922 | 5 -1.919 | 97.746 | 1.00 23.60 |
| ATOM | | E2 PHE B 200 | 53.229 | | 96.938 | 1.00 27.63 |
| ATOM | | Z PHE B 200 | 52.182 | | 97.547 97.143 | 1.00 23.56 |
| ATOM | 4606 C | | 51.296 | | 96.658 | 1.00 28.37 1.00 25.51 |
| ATOM | 4607 O | PHE B 200 | 52.112 | | 97.167 | 1.00 20.92 |
| ATOM | 4608 N | | 50.094 | | 96.252 | 1.00 27.41 |
| MOTA | 4609 C | | 49.576 | -7.972 | 96.454 | 1.00 31.98 |
| MOTA | 4610 CI | | 48.056 | | 96.487 | 1.00 31.57 |
| MOTA | 4611 C | | 47.486 | | 97.449 | 1.00 39.17 |
| ATOM ATOM | 4612 CI 4613 OI | D GLU B 201 E1 GLU B 201 | 45.987 | | 97.316 | 1.00 40.31 |
| ATOM | | E2 GLU B 201 | 45.332 45.475 | | 97.500 | 1.00 38.90 |
| ATOM | 4615 C | GLU B 201 | 49.979 | | 97.019 95.422 | 1.00 35.04 |
| ATOM | 4616 O | GLU B 201 | | -10.219 | 95.690 | 1.00 30.83 1.00 26.34 |
| MOTA | 4617 N | | 50.362 | | 94.234 | 1.00 24.95 |
| ATOM | 4618 CA | LYS B 202 | 50.764 | -9.501 | 93.195 | 1.00 22.79 |
| MOTA | 4619 CE | | 49.588 | | 92.258 | 1.00 25.12 |
| MOTA | 4620 CC | | | -10.523 | 93.000 | 1.00 35.38 |
| MOTA | 4621 CI | | 47.431 | -11.099 | 92.103 | 1.00 38.67 |
| ATOM ATOM | 4622 CE 4623 NZ | | 46.498 | -11.998 | 92.903 | 1.00 40.98 |
| ATOM | 4624 C | LYS B 202 LYS B 202 | | -12.659 | 92.028 | 1.00 46.65 |
| MOTA | 4625 O | LYS B 202 | 51.975 52.355 | -9.007 -7.838 | 92.435 | 1.00 24:62 |
| ATOM | 4626 N | GLY B 203 | 52.598 | -7.838 -9.910 | 92.549 91.684 | 1.00 21.83 1.00 17.60 |
| ATOM | 4627 CA | - | 53.779 | -9.545 | 90.928 | 1.00 17.80 |
| ATOM | 4628 C | GLY B 203 | | -10.297 | 91.396 | 1.00 20.36 |
| MOTA | 4629 O | GLY B 203 | | -10.070 | 90.888 | 1.00 23.83 |
| ATOM | 4630 N | PHE B 204 | 54.855 | -11.201 | 92.358 | 1.00 24.82 |
| ATOM | 4631 CA | | | -11.957 | 92.859 | 1.00 24.24 |
| ATOM | 4632 CB | PHE B 204 | | -12.567 | 94.236 | 1.00 22.72 |
| ATOM | 4633 CG | PHE B 204 | | -11.549 | 95.322 | 1.00 25.26 |
| ATOM ATOM | 4634 CD: 4635 CD: | 1 PHE B 204 2 PHE B 204 | | -10.977 | 95.535 | 1.00 23.80 |
| ATOM | | 1 PHE B 204 | | -11.159 | 96.133 | 1.00 20.25 |
| ATOM | 4637 CE2 | | | -10.036 -10.221 | 96.545 97.141 | 1.00 29.98 |
| ATOM | 4638 CD | PHE B 204 | 55.124 | -10.221 | 97.350 | 1.00 24.40 1.00 25.54 |
| ATOM | 4639 C | PHE B 204 | 56.412 | | 91.894 | 1.00 25.34 |
| ATCM | 4640 O | PHE B 204 | 55.613 | -13.540 | 91.091 | 1.00 20.65 |
| ATOM | 4641 N | LEU B 205 | 57.676 | -13.449 | 91.986 | 1.00 24.25 |
| ATOM | 4642 CA | LEU B 205 | 58.233 | -14.472 | 91.114 | 1.00 30.66 |
| ATOM | 4643 CB | LEU B 205 | 59 .723 | -14.637 | 91.413 | 1.00 34.01 |
| • | 4 | A E R III | | - | - | |

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Figure 18-71

| ATOM | 4644 | CG | LEU B 2 | 205 | 60.495 | -15.669 | 90.592 | 1.00 34.12 |
|------|-------|-----|---------|-----|--------|---------|--------|------------|
| ATOM | 4645 | CD1 | LEU 3 2 | 205 | 60.356 | -15.382 | 89.109 | 1.00 32.95 |
| ATOM | 4646 | CD2 | LEU B 2 | 205 | 61.957 | -15.629 | 91.005 | 1.00 36.49 |
| ATOM | 4647 | Ċ | LEU B 2 | | 57.535 | -15.827 | 91.205 | 1.00 30.51 |
| ATOM | 4648 | ō | LEU B 2 | | 57.467 | -16.562 | 90.220 | 1.00 25.89 |
| | 4649 | N | GLU B 2 | | 57,010 | -16.147 | 92.382 | 1.00 30.43 |
| ATOM | 4650 | CA | GLU B 2 | | | -17.423 | 92,605 | 1.00 30.64 |
| ATOM | 4651 | CB | GLU B 2 | | | -17.601 | 94.093 | 1.00 34.77 |
| MOTA | | | GLU B 2 | | | -17.512 | 95.033 | 1.00 42.50 |
| MOTA | 4652 | CG | | | | -16.084 | 95.270 | 1.00 45.76 |
| ATOM | 4653 | CD | GLU B 2 | | | -15.438 | 94.333 | 1.00 42.62 |
| ATOM | 4654 | | GLU B 2 | | | | | 1.00 50.22 |
| ATOM | 4655 | | GLU B 2 | | | -15.602 | 96.413 | 1.00 30.22 |
| ATOM | 4656 | С | GLU B 2 | | | -17.587 | 91.811 | |
| ATOM | 4657 | 0 | GLU B 2 | | | -18.708 | 91.563 | 1.00 28.18 |
| MOTA | 4658 | N | | 207 | | -16.472 | 91.425 | 1.00 25.16 |
| ATOM | 4659 | CA | GLU B 2 | 207 | | -16.499 | 90.664 | 1.00 28.78 |
| ATOM | 4660 | CB | GLU B 2 | 207 | | -15.107 | 90.695 | 1.00 30.76 |
| ATOM | 4661 | CG | GLU B 2 | 207 | | -14.659 | 92.093 | 1.00 29.39 |
| ATOM | 4662 | CD | GLU B 2 | 207 | 52.057 | -13.151 | 92.230 | 1.00 27.87 |
| ATOM | 4663 | OE1 | GLU B 2 | 207 | 51.656 | -12.477 | 91.261 | 1.00 24.38 |
| MOTA | 4664 | OE2 | | | 52.389 | -12.636 | 93.316 | 1.00 25.36 |
| MOTA | 4665 | C | GLU B 2 | | 53.453 | -16.922 | 89.224 | 1.00 29.48 |
| MOTA | 4666 | ō | GLU B 2 | | 53.658 | -16.077 | 88.351 | 1.00 27.48 |
| ATOM | 4667 | N | ILE B 2 | | 53.442 | -18.230 | 88.976 | 1.00 26.67 |
| | 4668 | CA | | 208 | | -18.754 | 87.646 | 1.00 32.60 |
| ATOM | 4669 | CB | ILE B 2 | | | -19.877 | 87.740 | 1.00 34.26 |
| ATOM | 4670 | CG2 | _ | 208 | | -20.296 | 86.352 | 1.00 41.65 |
| ATOM | - | CG1 | ILE B 2 | | | -19.404 | 88.532 | 1.00 36.07 |
| MOTA | 4671 | CD1 | | | | -18.338 | 87.851 | 1.00 45.18 |
| ATOM | 4672 | | ILE B 2 | | | -19.289 | 86.870 | 1.00 32.26 |
| ATOM | 4673 | C | ILE B 2 | | | -19.799 | 85.759 | 1.00 27.43 |
| MOTA | 4674 | 0 | | 209 | | ~19.165 | 87.442 | 1.00 32.60 |
| ATOM | 4675 | N | | | | -19.652 | 86.760 | 1.00 35.07 |
| MOTA | 4676 | CA | GLY B 2 | | | | 87.420 | 1.00 36.19 |
| MOTA | 4677 | С | | 209 | | -20.892 | 88.235 | 1.00 31.61 |
| ATOM | 4678 | 0 | GLY B | | | -21.524 | 87.066 | 1.00 36.98 |
| ATOM | 4679 | N | | 210 | | -21.245 | 87.647 | 1.00 40.60 |
| MOTA | 4680 | CA | GLU B 2 | | | -22.412 | 88.672 | 1.00 37.98 |
| ATOM | 4681 | CB | GLU B 2 | | | -21.964 | | 1.00 42.78 |
| ATOM | 4682 | CG | GLU B | | | -21.234 | 88.058 | 1.00 48.41 |
| ATOM | 4683 | CD | GLU B 2 | | | -20.717 | 89.098 | 1.00 51.03 |
| ATOM | 4684 | OE1 | | | | -20.202 | 88.709 | |
| ATOM | 4685 | OE2 | | | | -20.814 | 90.306 | 1.00 49.90 |
| ATOM | 4686 | С | GLU B 2 | | | -23.248 | 86.564 | 1.00 39.48 |
| ATOM | 4687 | 0 | GLU B 2 | | | -22.751 | 85.471 | 1.00 33.65 |
| ATOM | 4.688 | N | GLY B 2 | | 46.736 | -24.515 | 86.876 | 1.00 39.18 |
| ATOM | 4689 | CA | GLY B 2 | 211 | 46.087 | -25.399 | 85.923 | 1.00 38.43 |
| ATOM | 4690 | С | GLY B 2 | 211 | 46,877 | -25.500 | 84.637 | 1.00 40.29 |
| ATOM | 4691 | 0 | GLY B 2 | | 48.101 | -25.610 | 84.666 | 1.00 39.39 |
| ATOM | 4692 | N | LYS B 2 | 212 | | -25.458 | 83.504 | 1.00 40.90 |
| MOTA | 4693 | CA | LYS B | 212 | 46.864 | -25.538 | 82.219 | 1.00 43.53 |
| ATOM | 4694 | CB | LYS B 2 | 212 | | -25.548 | 81.080 | 1.00 47.87 |
| ATOM | 4695 | CG | LYS B 2 | 212 | 44.795 | -26.665 | 81.144 | 1.00 53.09 |
| ATOM | 4696 | CD | LYS B 1 | 212 | 45.398 | -28.076 | 81.130 | 1.00 58.61 |
| ATOM | 4697 | CE | LYS B 2 | 212 | 46.069 | -28.454 | 82.452 | 1.00 59.78 |
| | 4698 | NZ | LYS B 2 | 212 | | -29.825 | 82.420 | 1.00 62.17 |
| ATOM | 4699 | C | LYS B | 212 | 47.823 | -24.363 | 82.040 | 1.00 38.84 |
| ATOM | 4700 | 0 | LYS B | 212 | 48 797 | -24.457 | 81.295 | 1.00 40.33 |
| ATOM | | | GLY B | 213 | 47.543 | -23.262 | 82.731 | 1.00 37.20 |
| MOTA | 4701 | N | | | 48.384 | -22.081 | 82.627 | 1.00 34.66 |
| MOTA | 4702 | CA | GLY B 2 | | 49.625 | -22.107 | 83.505 | 1.00 37.09 |
| ATOM | 4703 | C | | | | -21.165 | 83.489 | 1.00 25.85 |
| ATOM | 4704 | 0 | GLY B | | | -23.180 | 84.273 | 1.00 33.33 |
| ATOM | 4705 | N | LYS B | | | | 85.148 | 1.00 37.90 |
| MOTA | 4706 | CA | LYS B 2 | | 50.953 | -23.297 | 85.954 | 1.00 38.89 |
| ATCM | 4707 | CB | LYS B | | 50.886 | -24.598 | 86.938 | 1.00 39.29 |
| ATOM | 4708 | CG | LYS B | C14 | | -24.786 | | 1.00 43.60 |
| ATCM | 4709 | CD | LYS B | 214 | 51.876 | -26.094 | 87.704 | 1.00 93.00 |

Figure 18-72

| MOTA | 4710 |) CE LYS B 214 | 53.04 | 7 -26.334 | 88.640 | 1.00 47.36 |
|------|------|----------------|--------|------------|---------|-------------|
| MOTA | 4713 | | 53 16 | 5 -25.264 | 89.666 | |
| MOTA | 4712 | | | | | |
| | | | 32.20 | 9 -23.275 | 84.291 | 1.00 34.16 |
| MOTA | 4713 | | | 4 -24.136 | 83.438 | 1.00 34.70 |
| MOTA | 4714 | N GLY B 215 | 53.05 | 7 -22.279 | 84.523 | 1.00 33.58 |
| MOTA | 4715 | CA GLY B 215 | | 5 -22.152 | 83.743 | 1.00 28.27 |
| MOTA | 4716 | | | | | |
| | | | | 4 -21.155 | 82.605 | 1.00 31.02 |
| ATOM | 4717 | | 55.03 | 3 -20.911 | 81.833 | 1.00 23.68 |
| ATOM | 4718 | N TYR B 216 | 52.91 | 3 - 20.564 | 82.493 | 1.00 22.45 |
| MOTA | 4719 | | | 3 -19.605 | 81.426 | |
| ATOM | 4720 | | | | | 1.00 24.03 |
| | | | 51.45 | 3 -20.013 | 80.603 | 1.00 17.60 |
| MOTA | 4721 | | 51.68 | 2 -21.291 | 79.806 | 1.00 25.96 |
| ATOM | 4722 | CD1 TYR B 216 | 51.692 | 2 -22.538 | 80.435 | 1.00 21.41 |
| MOTA | 4723 | CE1 TYR B 216 | 51 989 | -23.704 | 79.729 | 1.00 23.78 |
| ATOM | 4724 | CD2 TYR B 216 | 51.50 | 22.709 | | |
| | | | | -21.242 | 78.439 | 1.00 19.62 |
| MOTA | 4725 | CE2 TYR B 216 | | -22.402 | 77.72-2 | 1.00 26.39 |
| MOTA | 4726 | CZ TYR B 216 | 52.27 | -23.630 | 78.379 | 1.00 29.35 |
| ATOM | 4727 | OH TYR B 216 | | -24.782 | 77.690 | 1.00 27.75 |
| ATOM | 4728 | C TYR B 216 | | -18.153 | | |
| | | | | | 81.884 | 1.00 24.53 |
| ATOM | 4729 | O TYR B 216 | 52.065 | -17.298 | 81.159 | 1.00 18.99 |
| ATOM | 4730 | N ASN B 217 | 53.052 | -17.886 | 83.098 | 1.00 21.41 |
| ATOM | 4731 | CA ASN B 217 | | -16.534 | 83.642 | 1.00 21.23 |
| ATOM | 4732 | CB ASN B 217 | | -16.325 | | |
| | 4733 | | | | 84.669 | 1.00 16.78 |
| MOTA | | CG ASN B 217 | | -14.889 | 85.162 | 1.00 22.07 |
| MOTA | 4734 | OD1 ASN B 217 | 52.506 | -14.521 | 86.163 | 1.00 23.13 |
| ATOM | 4735 | ND2 ASN B 217 | 51.146 | -14.058 | 84.435 | 1.00 19.26 |
| ATOM | 4736 | C ASN B 217 | | -16.339 | 84.291 | 1.00 19.40 |
| ATOM | 4737 | O ASN B 217 | | | | |
| | 4738 | | 54.65/ | -17.145 | 85.124 | 1.00 19.28 |
| ATOM | | N LEU B 218 | 55.130 | -15.273 | 83.905 | 1.00 18.65 |
| ATOM | 4739 | CA LEU B 218 | 56.459 | -15.004 | 84.444 | 1.00 16.41 |
| ATOM | 4740 | CB LEU B 218 | 57.512 | -15.244 | 83.368 | 1.00 18.29 |
| ATOM | 4741 | CG LEU B 218 | | -15.872 | 83.782 | 1.00 28.15 |
| ATOM | 4742 | CD1 LEU B 218 | 59.873 | 15.0.2 | | |
| | | | 39.073 | -15.563 | 82.695 | 1.00 20.50 |
| MOTA | 4743 | CD2 LEU B 218 | | -15.348 | .85.116 | 1.00 22.53 |
| ATOM | 4744 | C LEU B 218 | 56.595 | -13.562 | 84.926 | 1.00 17.89 |
| ATOM | 4745 | O LEU B 218 | | -12.627 | 84.128 | 1.00 14.48 |
| ATOM | 4746 | N ASN B 219 | | -13.395 | 86.219 | 1.00 14.09 |
| ATOM | 4747 | CA ASN B 219 | | | | |
| | | | | -12.075 | 86.821 | 1.00 18.41 |
| MOTA | 4748 | CB ASN B 219 | | -11.922 | 88.111 | 1.00 14.64 |
| ATOM | 4749 | CG ASN B 219 | 54.748 | -11.898 | 87.868 | 1.00 27.12 |
| ATOM | 4750 | OD1 ASN B 219 | | -11.332 | 86.880 | 1.00 20.21 |
| ATOM | 4751 | ND2 ASN B 219 | 52 002 | -12.480 | 88.787 | |
| | 4752 | | 55.562 | -12.400 | | 1.00 23.62 |
| ATOM | | | | -11.843 | 87.172 | 1.00 20.39 |
| ATOM | 4753 | O ASN B 219 | 59.115 | -12.672 | 87.841 | 1.00 20.41 |
| MOTA | 4754 | N ILE B 220 | 59.056 | -10.717 | 86.729 | 1.00 15.11 |
| ATOM | 4755 | CA ILE B22C | | -10.394 | 87.033 | 1.00 17.16 |
| ATOM | 4756 | CB ILE B 220 | 61 250 | -10.083 | | |
| | | | | | 85.740 | 1.00 20.78 |
| ATOM | 4757 | CG2 ILE B 22C | 62.736 | -9.821 | 86.094 | 1.00 18.08 |
| MOTA | 4758 | CG1 ILE B 220 | 61.138 | -11.250 | 84.748 | 1.00 17.62 |
| ATOM | 4759 | CD1 ILE B 220 | 61.646 | -12.590 | 85.273 | 1.00 20.72 |
| ATOM | 4760 | C ILE B 220 | | -9.161 | 87.947 | 1.00 21.17 |
| | 4761 | | | | | |
| MOTA | | | 60.565 | -8.036 | | .1.00 16.03 |
| ATOM | 4762 | N PRO B 221 | 60.367 | -9.357 | 89.274 | 1.00 21.74 |
| MOTA | 4763 | CD PRO B 221 | 60.135 | -10.619° | 90.000 | 1.00 22.96 |
| ATOM | 4764 | CA PRO B 221 | 60.394 | -8.225 | 90.213 | 1.00 19.16 |
| ATOM | 4765 | CB PRO B 221 | 59.947 | | 91.523 | |
| | | | | -8.869 | | 1.00 19.40 |
| ATOM | 4766 | CG PRO B 221 | 60.564 | -10.251 | 91.407 | 1.00 23.02 |
| ATOM | 4767 | C PRO B 221 | 61.799 | -7.634 | 90.289 | 1.00 22.42 |
| MOTA | 4768 | O PRO B 221 | 62.780 | -8.369 | 90.425 | 1.00 20.71 |
| ATOM | 4769 | N LEU B 222 | 61.899 | -6.309 | 90.202 | 1.00 22.74 |
| ATOM | 4770 | CA LEU B 222 | | | | |
| | | | 63.198 | -5.643 | 90.223 | 1.00 21.18 |
| ATOM | 4771 | CB LEU B 222 | 63.453 | -4.993 | 88.850 | 1.00 17.21 |
| ATOM | 4772 | CG LEU B 222 | 63.467 | -6.027 | 87.721 | 1.00 20.26 |
| ATCM | 4773 | CD1 LEU B 222 | 63.453 | -5.354 | 86.361 | 1.00 20.00 |
| ATCM | 4774 | CD2 LEU B 222 | 64.696 | | 87.881 | 1.00 21.93 |
| | 4775 | C LEU B 222 . | 63.335 | | _ | |
| ATOM | 4,,, | C 1100 B 222 . | 03.335 | -4.616 | 91.353 | 1.00 20.04 |

Figure 18-73

| | | | | | | | | 3 00 17 ED |
|-------------------|-------------|------|------------|---|--------|--------|----------|------------|
| MOTA | 4776 | 0 | LEU B 222 | | 62.350 | -4.030 | 91.806 | 1.00 17.58 |
| | | N | PRO B 223 | | 64.571 | -4.394 | 91.830 . | 1.00 19.48 |
| ATOM | 4777 | | | | 65.806 | -5.072 | 91.400 | 1.00 16.80 |
| $MOT \mathcal{L}$ | 4778 | CD | PRO B 223 | | | | | 1.00 20.38 |
| MOTA | 4779 | CA | PRO B 223 | | 64.873 | -3.454 | 92.915 | |
| ATOM | 4780 | CB | PRO B 223 | | 66.274 | -3.881 | 93.327 | 1.00 26.11 |
| | | CG | PRO B 223 | | 66.884 | -4.161 | 91.973 | 1.00 19.74 |
| MOTA | 4781 | | PRO D 223 | | 64.818 | -1.971 | 92.553 | 1.00 21.39 |
| ·ATOM | 4782 | С | PRO B 223 | | | | | 1.00 17.16 |
| MOTA | 4783 | C | PRO B 223 | | 64.815 | -1.598 | 91.380 | |
| ATOM | 4784 | N | LYS B 224 | | 64.798 | -1.142 | 93.589 | 1.00 20.65 |
| • | | | LYS B 224 | | 64.755 | 0.311 | 93.462 | 1.00 27.00 |
| MOTA | 4785 | | PI3 D 224 | | 64.577 | 0.938 | 94.844 | 1.00 36:47 |
| ATOM | 4786 | CB | LYS B 224 | | | | | 1.00 37.72 |
| ATOM | 4787 | CG | LYS .B 224 | | 63.415 | 0.389 | 95.651 | |
| ATOM | 4788 | CD | LYS B 224 | • | 63.541 | 0.833 | 97.101 | 1.00 42.06 |
| | | CE | LYS B 224 | | 62.420 | 0.276 | 97.955 | 1.00 45.18 |
| ATOM . | 4789 | | | | 62.645 | 0.570 | 99.399 | 1.00 46.30 |
| ATOM | 4790 | ΝZ | LYS B 224 | | | | 92.874 | 1.00 27.01 |
| MOTA | 4791 | С | LYS B 224 | • | 66.071 | 0.808 | | |
| ATOM | 4792 | 0 | LYS B 224 | | 67.098 | 0.139 | 92.995 | 1.00 21.54 |
| | 4793 | N | GLY B 225 | | 66.038 | 1.989 | 92.259 | 1.00 22.66 |
| MOTA | | | GLY B 225 | | 67.239 | 2.565 | 91.669 | 1.00 25.67 |
| MOTA | 4794 | CA | GLY B 223 | | | 1.809 | 90.459 | 1.00 24.95 |
| MOTA | 4795 | С | GLY B 225 | | 67.768 | | | 1.00 26.83 |
| ATOM | 4796 | Ö | GLY B 225 | | 68.917 | 1.975 | 90.069 | |
| | 4797 | N | LEU B 226 | | 66.926 | 0.980 | 89.855 | 1.00 21.79 |
| ATOM | | | LEU B 226 | | 67.319 | 0.180 | 88.692 | 1.00 22.91 |
| ATOM | 4798 | CA | | | 66.067 | -0.473 | 88.099 | 1.00 23.29 |
| ATOM | 4799 | CB | LEU B 226 | | | | 87.091 | 1.00 26.71 |
| ATOM | 4800 | CG | LEU B 226 | | 66.238 | -1.605 | | |
| ATOM | 4801 | CD1 | LEU B 226 | | 66.846 | -2.804 | 87.813 | 1.00 26.44 |
| | 4802 | | LEU B 226 | | 64.877 | -1.997 | 86.508 | 1.00 22.96 |
| ATOM | | | | | 68.008 | 1.017 | 87.603 | 1.00 22.66 |
| MOTA | 4803 | C | | | | 2.087 | 87.250 | 1.00 20.19 |
| ATOM | 4804 | 0 | LEU B 226 | | 67.517 | | | 1.00 15.52 |
| ATOM | 4805 | N | ASN B 227 | | 69.134 | 0.549 | 87.060 | 1.00 15.52 |
| ATOM | 4806 | CA | ASN B 227 | | 69.794 | 1.317 | 85.998 | 1.00 19.49 |
| | | CB | ASN B 227 | | 71.304 | 1.474 | 86,270 | 1.00 20.43 |
| MOTA | 4807 | | | | 72.062 | 0.161 | 86.206 | 1.00 28.97 |
| MOTA | 4808 | CG | ASN B 227 | | | | 85.199 | 1.00 24.30 |
| ATOM | 4809 | OD1 | | | 72.015 | -0.546 | 65.133 | |
| ATOM | 4810 | ND2 | ASN B 227 | | 72.786 | -0.160 | 87.276 | 1.00 20.88 |
| | 4811 | C | ASN B 227 | | 69.548 | 0.671 | 84.630 | 1.00 21.26 |
| ATOM | | | | | 69.004 | -0.432 | 84.555 | 1.00 18.90 |
| ATOM | 4812 | 0 | | | | 1.347 | 83.552 | 1.00 20.98 |
| MOTA | 4813 | N | ASP B 228 | | 69.949 | | | 1.00 22.61 |
| MOTA | 4814 | CA | ASP B 228 | | 69.720 | 0.817 | 82.208 | 1.00 23.46 |
| ATOM | 4815 | CB | ASP B 228 | | 70.270 | 1.753 | 31.126 | |
| | | CG | ASP 3 228 | | 69.596 | 3.113 | 81.119 | 1.00 26.12 |
| ATOM | 4816 | | | | 68.387 | 3.193 | 81.415 | 1.00 26.75 |
| MOTA | 4817 | OD1 | ASP B 220 | | | 4.101 | 80.773 | 1.00 30.22 |
| ATOM | :818 | OD2 | | | 70.276 | | | 1.00 23.49 |
| ATOM | 4819 | С | ASP B 228 | | 70.286 | -0.573 | 81.952 | |
| | 4820 | o | ASP B 228 | | 69.651 | -1.390 | 81.288 | 1.00 19.31 |
| ATOM | | N | ASN B 229 | | 71.484 | -0.836 | 82,453 | 1.00 22.24 |
| ATCM | 4821 | | | | 72.111 | -2.135 | 82,250 | 1.00 23.30 |
| ATOM | 4822 | CA | ASN B 229 | | | | 82.737 | 1.00 20.99 |
| ATOM | 4823 | CB · | ASN B 229 | | 73.562 | -2.101 | | 1.00 25.71 |
| TOM | 4824 | CG | ASN B 229 | | 74.441 | -1.237 | 81.859 | |
| | 4825 | ODI | ASN B 229 | | 74.644 | -1.538 | 80.678 | 1.00 26.40 |
| ATOM | | | | | 74.955 | -0.151 | 82.417 | 1.00 27.44 |
| ATOM | 4826 | | ASN B 229 | | | | 82.943 | 1.00 23.74 |
| ATCM | 4827 | С | ASN B 229 | | 71.341 | -3.252 | 02.743 | 1.00 20.51 |
| ATOM | 4828 | 0 | ASN B 229 | | 71.207 | -4.346 | 82.402 | 1.00 20.51 |
| | 4829 | N | GLU B 230 | | 70.832 | -2.976 | 84.139 | 1.00 23.06 |
| ATOM | | | GLU B 230 | | 70.069 | -3.977 | 84.874 | 1.00 23.01 |
| MOTA | 4830 | CA | | | 69.799 | -3.480 | 86.297 | 1.00 24.73 |
| ATOM | 4831 | CB | GLU B 230 | | | | 87.087 | 1.00 27.28 |
| MOTA | 4832 | ÇG | GLU B 230 | | 71.069 | -3.201 | | 1.00 27.20 |
| | 4833 | CD | GLU B 230 | | 70.792 | -2.649 | 88.470 | 1.00 27.47 |
| ATOM | | OE1 | | | 70.086 | -1.625 | 88.569 | 1.00 27.87 |
| ATOM | 4834 | OFT | 0111 7 220 | | 71.286 | -3.232 | 89.455 | 1.00 26.79 |
| ATOM | 4835 | | GLU B 230 | | | | 84.146 | 1.00 24.25 |
| ATOM | 4836 | С | GLU B 230 | | 68.749 | -4.281 | | 1.00 15.89 |
| ATCM | 4837 | 0 | GLU B 230 | | 68.347 | -5.445 | 84.022 | 1.00 13.05 |
| | | N | PHE B 231 | | 68.091 | -3.242 | 83.637 | 1.00 21.46 |
| ATCM | 4838 | | PHE B 231 | | 66.814 | -3.429 | 82.933 | 1.00 22.84 |
| ATOM | 4839 | CA | | | | -2.079 | | 1.00 23.96 |
| ATOM | 4840 | CB | PHE B 231 | | 66.210 | | | |
| ATOM | 4841 | CG | PHE B 231 | | 64.803 | -2.182 | 81.975 | 1.00 20.20 |
| - O12 | | | | | | | | |

| MOTA | 4842 | CD1 | .PHE B | 231 | 63.738 | -2.514 | 82.805 | 1.00 25.00 |
|------|------|-----|--------|-----|----------------|---------|-------------------------------|------------|
| | | | | | | | | |
| MOTA | 4843 | CD2 | | | 64.550 | -1.956 | 80.627 | 1.00 22.93 |
| ATOM | 4844 | CE: | PHE E | 231 | 62.440 | -2.618 | 82.304 | 1.00 25.03 |
| | | CE2 | | | 63.250 | -2.059 | 80.114 | 1.00 27.46 |
| MOTA | 4845 | | | | | | | |
| MOTA | 4846 | CZ | PHE B | 231 | 62.196 | -2.390 | 80.957 | 1.00 20.25 |
| | 4847 | С | PHE B | 231 | 66.978 | -4.288 | 81.677 | 1.00 23.14 |
| MOTA | | | | | | | | |
| ATOM | 4848 | 0 | PHE B | 231 | 66.221 | -5.239 | 81.464 | 1.00 20.02 |
| ATOM | 4849 | N | LEU B | 222 | 67.963 | -3.952 | 80.845 | 1.00 22.02 |
| | | | | | | | | |
| MOTA | 4850 | CA | LEU B | 232 | 68.200 | -4.697 | 79.614 | 1.00 19.97 |
| MOTA | 4851 | CB | LEU B | 232 | 69.192 | -3.942 | 78.734 | 1.00 24.99 |
| | | | | | | | | |
| ATOM | 4852 | CG | LEU B | 232 | 68.665 | -2.581 | 78.263 | 1.00 29.73 |
| MOTA | 4853 | CD1 | LEU B | 232 | 69.746 | -1.856 | 77.454 | 1.00 28.11 |
| | | CD2 | | | | | 77.414 | |
| MOTA | 4854 | | | | 67.409 | -2.784 | | 1.00 26.54 |
| ATOM | 4855 | С | LEU B | 232 | 68.688 | -6.119 | 79.898 | 1.00 19.25 |
| ATOM | 4856 | 0 | LEU B | 232 | 68.365 | ~7.051 | 79.162 | 1.00 19.49 |
| | | | | | | | | |
| MOTA | 4857 | N | PHE B | 233 | 69.468 | -6.280 | 80.962 | 1.00 20.50 |
| ATOM | 4858 | CA | PHE .B | 233 | 69.950 | -7.599 | 81.378 | 1.00 20.70 |
| | | | | | | | | |
| MOTA | 4859 | CB | PHE B | 233 | 70.825 | -7.471 | 82.632 | 1.00 23.75 |
| MOTA | 4860 | CG | PHE B | 233 | 71.217 | -8.790 | 83.239 | 1.00 28.58 |
| | | | | | 72.285 | -9.519 | 82.731 | 1.00 30.48 |
| MOTA | 4861 | CD1 | | | | | | |
| MOTA | 4862 | CD2 | PHE B | 233 | 70.481 | -9.328 | 84.294 | 1.00 25.32 |
| | 4863 | CE1 | PHE B | 223 | 72 617 | -10.762 | 83.262 | 1.00 31.87 |
| ATOM | | | | | | | | |
| MOTA | 4864 | CE2 | PHE B | 233 | 70.803 | -10.573 | 84.832 | 1.00 31.26 |
| ATOM | 4865 | CZ | PHE B | 233 | 71.871 | -11.292 | 84.317 | 1.00 32.29 |
| | | | | | | | 81.727 | |
| MOTA | 4866 | С | PHE B | | 68.712 | -8.439 | | 1.00 20.23 |
| MOTA | 4867 | 0 | PHE B | 233 | 68.553 | -9.567 | 81.270 | 1.00 21.56 |
| | 4868 | N | ALA B | 234 | 67.842 | -7.878 | 82.560 | 1.00 21.26 |
| MOTA | | | | | | | | |
| MOTA | 4869 | CA | ALA B | 234 | . 66.626 | -8.576 | 82.963 | 1.00 19.60 |
| ATOM | 4870 | CB | ALA B | 234 | 65.835 | -7.733 | 83.950 | 1.00 19.25 |
| | | | | | | | 81.749 | 1.00 18.87 |
| MOTA | 4871 | С | ALA B | | 65.772 | -8.898 | | |
| MOTA | 4872 | 0 | ALA B | 234 | 65.253 | -10.010 | 81.624 | 1.00 21.91 |
| ATOM | 4873 | N | LEU B | 235 | 65.634 | -7.934 | 80.845 | 1.00 20.29 |
| | | | | | | | • | |
| MOTA | 4874 | CA | LEU B | 235 | 64.822 | -8.141 | 79.652 | 1.00 19.53 |
| ATOM | 4875 | CB | LEU B | 235 | 64.773 | -6:874 | 78 ⁻ . 79 5 | 1.00 24.07 |
| | | | | | | -6.607 | 78.024 | 1.00 27.87 |
| MOTA | 4876 | CG | LEU B | | 63.465 | | | |
| ATOM | 4877 | CD1 | LEU B | 235 | 63.783 | -5.813 | 76.770 | 1.00 20.77 |
| ATOM | 4878 | CD2 | LEU B | 235 | 62.761 | -7.897 | 77.664 | 1.00 26.94 |
| | | | | | | | 78.795 | 1.00 20.79 |
| ATOM | 4879 | С | LEU B | | 65.376 | -9.276 | | |
| ATOM | 4880 | 0 | LEU B | 235 | 64.648 | -10.205 | 78.431 | 1.00 18.25 |
| ATOM | 4881 | N | GLU B | 236 | 66.665 | -9.191 | 78.462 | 1.00 19.33 |
| | • | | | | | | | |
| ATOM | 4882 | ca | GLU B | 236 | 67.303 | -10.206 | 77.629 | 1.00 27.93 |
| MOTA | 4883 | CB | GLU B | 236 | 68.777 | -9.853 | 77.384 | 1.00 31.06 |
| | | | GLU B | | 68.969 | -8.597 | 76.548 | 1.00 43.60 |
| MOTA | 4884 | CG | | | | | | |
| ATOM | 4885 | CD | GLU B | 236 | 70.428 | -8.292 | 76.259 | 1.00 45.19 |
| ATOM | 4886 | OFI | GLU B | 236 | 70.697 | -7.309 | 75.538 | 1.00 48.77 |
| | | | | | | | | |
| ATOM | 4887 | OE2 | GLU B | 436 | 71.30 <i>c</i> | -9.032 | 76.751 | 1.00 52.72 |
| ATOM | 4888 | С | GLU B | 236 | 67.20. | -11.607 | 78.209 | 1.00 24.89 |
| | | ŏ | GLU B | | 66.865 | -12.552 | 77.501 | 1.00 22.06 |
| MOTA | 4889 | | | | | | | |
| MOTA | 4890 | N | LYS B | 237 | 67.520 | -11.748 | 79.492 | 1.00 24.20 |
| MOTA | 4891 | CA | LYS B | 237 | 67 449 | -13.058 | 80.130 | 1.00 27.10 |
| | | | | | | | | |
| ATOM | 4892 | CB | LYS B | 231 | 67.989 | -12.984 | 81.562 | 1.00 23.43 |
| MOTA | 4893 | CG | LYS B | 237 | 69.466 | -12.641 | 81.650 | 1.00 29.46 |
| | | | LYS B | | | -13.683 | 80.924 | 1.00 31.65 |
| MOTA | 4894 | CD | | | | | | |
| MOTA | 4895 | CE | LYS B | 237 | 71.782 | -13.356 | 80.993 | 1.00 39.70 |
| ATOM | 4896 | NZ | LYS B | | 72 580 | -14.363 | 80.242 | 1.00 46.74 |
| | | | | | | | | |
| MOTA | 4897 | C | LYS B | | | -13.615 | 80.143 | 1.00 30.92 |
| MOTA | 4898 | 0 | LYS B | 237 | 65.789 | -14.766 | 79.763 | 1.00 31.42 |
| | | | | | | -12.806 | 80.573 | 1.00 25.86 |
| ATOM | 4899 | N | SER B | | | | | 1.00 23.00 |
| MOTA | 4900 | CA | SER B | 238 | 63.677 | -13.280 | 80.620 | 1.00 27.98 |
| | 4901 | | SER B | | | -12.241 | 81.289 | 1.00 23.89 |
| MOTA | | CB | | | | | | 1 00 20 27 |
| ATOM | 4902 | OG | SER B | 238 | 62.756 | -11.028 | 80.565 | 1.00 29.27 |
| ATOM | 4903 | С | | 238 | | -13.642 | 79.229 | 1.00 28.32 |
| | | | | | | -14.605 | 79.089 | 1.00 29.65 |
| HOTA | 1904 | 0 | SER B | 238 | | | | 1.00 23.03 |
| ATOM | 4905 | N | LEU B | 239 | 63.536 | -12.886 | 78.203 | 1.00 27.39 |
| | 4906 | CA | LEU B | 239 | | -13.192 | 76.846 | 1.00 32.52 |
| ATOM | | | | 222 | | | 75.837 | 1.00 30.53 |
| MOTA | 4907 | CB | LEU B | 233 | 03.344 | -12.129 | | 1.00 50.55 |

| ATOM | 4908 | CG | LEU I | 3 239 | 62.833 | -10.772 | 75.895 | 1.00 36.06 |
|--------|------|-----|---------|---------|----------|---------|--------|------------|
| | | | LEU I | | 63.404 | | 74.842 | 1.00 29.64 |
| MOTA | 4909 | | | | | | | |
| ATOM | 4910 | CD2 | LEU E | 3 239 | 61.338 | -10.976 | 75.667 | 1.00 30.73 |
| ATOM | 4911 | С | LEU I | 2 2 3 0 | . 63 500 | -14.563 | 76.430 | 1.00 34.15 |
| | | | | | | | | |
| MOTA | 4912 | 0 | LEU I | 3 239 | 62.879 | -15.340 | 75.803 | 1.00 33.23 |
| MOTA | 4913 | N | GLU F | 240 | 64.844 | -14.859 | 76.788 | 1.00 31.39 |
| | | | | | | | 76.472 | |
| ATOM | 4914 | CA | GLU I | | | -16.152 | | 1.00 33.79 |
| MOTA | 4915 | CB | GLU E | 3 240 | 66.859 | -16.238 | 77.011 | 1.00 38.51 |
| ATOM | 4916 | CG | GLU I | a. 240 | 67 878 | -15.407 | 76.275 | 1.00 40.56 |
| | | | | | | | | |
| ATOM | 4917 | CD | GLU E | 3 240 | 69.256 | -15.532 | 76.903 | 1.00 48.20 |
| MOTA | 4918 | OE1 | . GLU E | 240 | 69.685 | -16.679 | 77.161 | 1.00 45.36 |
| | | | | | | -14.492 | 77.130 | 1.00 48.21 |
| ATOM | 4919 | | GLU F | | | | | |
| ATOM | 4920 | С | GLU E | 3 240 | 64.604 | -17.258 | 77.108 | 1.00 33.23 |
| MOTA | 4921 | 0 | GLU E | 240 | 64.391 | -18.310 | 76.510 | 1.00 32.15 |
| | | | | | | | 78.331 | |
| ATOM | 4922 | Ŋ | ILE E | | | -17.017 | | 1.00 29.72 |
| MOTA | 4923 | CA | ILE E | 3 241 | 63.328 | -17.989 | 79.047 | 1.00 29.85 |
| ATOM | 4924 | CB | ILE F | | 63 006 | -17.489 | 80.466 | 1.00 30.42 |
| | | | | | | | | |
| MOTA | 4925 | CG2 | ILE E | 3 24 I | .62.049 | -18.456 | 81.162 | 1.00 29.88 |
| ATOM | 4926 | CG1 | ILE E | 241 | 64.309 | -17.311 | 81.254 | 1.00 29.77 |
| | | | | | 64.118 | -16.760 | 82.654 | 1.00 32.92 |
| ATOM | 4927 | CDI | | | | | | |
| MOTA | 4928 | C | ILE E | 241 | 62.016 | -18.247 | 78.298 | 1.00 34.65 |
| ATOM | 4929 | С | ILE E | 241 | 61.592 | -19.396 | 78.149 | 1.00 30.22 |
| | | | | | | -17.178 | 77.823 | 1.00 31.16 |
| ATOM | 4930 | N | VAL E | | | | | |
| ATOM | 4931 | CA | VAL E | 242 | 60.114 | -17.312 | 77.105 | 1.00 34.55 |
| ATOM | 4932 | CB | VAL E | 242 | 59.476 | -15.937 | 76.825 | 1.00 30.77 |
| | | | | | | -16.113 | 76.038 | 1.00 32.18 |
| ATOM | 4933 | CG1 | | | | | | |
| ATOM | 4934 | CG2 | VAL E | 242 | 59.201 | -15.214 | 78.140 | 1.00 31.57 |
| MOTA | 4935 | С | VAL E | 242 | 60.320 | -18.042 | 75.787 | 1.00 36.56 |
| | | | | | | | | |
| MOTA | 4936 | 0.7 | VAL E | | 59.572 | -18.959 | 75.453 | |
| ATOM | 4937 | N | LYS E | 243 | 61.337 | -17.627 | 75.042 | 1.00 38.64 |
| ATOM | 4938 | CA | LYS E | 243 | 61 659 | -18.241 | 73.760 | 1.00 44.36 |
| | | | | | | | | |
| ATOM | 4939 | CB | LYS E | 243 | | -17.659 | 73.214 | 1.00 48.33 |
| MOTA | 4940 | CG | LYS E | 243 | 62.810 | -16.399 | 72.386 | 1.00 53.88 |
| | 4941 | CD | LYS E | | 62 185 | -16.718 | 71.036 | 1.00 53.72 |
| MOTA | | | | | | | | |
| ATOM | 4942 | CE | LYS B | 243 | | -17.681 | 70.242 | 1.00 54.69 |
| ATOM | 4943 | NZ | LYS E | 243 | 62.456 | -18.025 | 68.923 | 1.00 57.75 |
| | 4944 | C | LYS B | | | -19.755 | 73.824 | 1.00 43.21 |
| MOTA | | | | | | | | |
| · ATOM | 4945 | 0 | LYS B | 243 | 61.432 | -20.455 | 72.884 | 1.00 42.92 |
| ATOM | 4946 | N | GLU B | 244 | 62.312 | -20.257 | 74.935 | 1.00 45.77 |
| | 4947 | CA | GLU B | | 62.528 | -21.687 | 75.085 | 1.00 47.72 |
| MOTA | | | | | | | | |
| MOTA | 4948 | CB | GLU B | 244 | 63.669 | -21.925 | 76.075 | 1.00 50.89 |
| MOTA | 4949 | CG | GLU B | 244 | 64.080 | -23.378 | 76.208 | 1.00 57.16 |
| | 4950 | CD | GLU B | | 65.223 | -23.564 | 77.173 | 1.00 57.74 |
| MOTA | | | | | | | | |
| ATOM | 4951 | CE1 | | | 66.295 | -22.967 | 76.942 | 1.00 60.18 |
| MOTA | 4952 | OE2 | GLU B | 244 | 65.049 | -24.308 | 78.160 | 1.00 61.59 |
| | 4953 | С | GLU B | 244 | 61.312 | -22.507 | 75.505 | 1.00 47.78 |
| ATOM | | | | | | | | |
| ATOM | 4954 | 0 | GLU B | | | -23.736 | 75.544 | 1.00 51.39 |
| ATOM | 4955 | N | VAL B | 245 | 60.200 | -21.851 | 75.805 | 1.00 43.31 |
| ATOM | 4956 | CA | VAL B | 245 | 59.019 | -22.589 | 76.230 | 1.00 43.55 |
| | | | | | | | | 1.00 45.89 |
| ATOM | 4957 | CB | VAL B | | | -22.514 | 77.771 | |
| ATOM | 4958 | CG1 | VAL B | 245 | . 57.665 | -23.322 | 78.231 | 1.00 49.90 |
| | 4959 | | VAL B | | | -23.040 | 78.435 | 1.00 46.37 |
| ATOM | | | | | | | | |
| MOTA | 4960 | С | VAL B | | | -22.115 | 75.565 | 1.00 41.01 |
| MOTA | 4961 | e | VAL B | 245 | 56.659 | -22.676 | 75.798 | 1.00 39.36 |
| | 4962 | N | PHE B | | | -21.101 | 74.716 | 1.00 34.37 |
| ATOM | | | | | | | | |
| ATOM | 4963 | CA | PHE B | | | -20.602 | 74.077 | 1.00 34.36 |
| ATOM | 4964 | CB | PHE B | 246 | 55.986 | -19.517 | 74.958 | 1.00 30.80 |
| | 4965 | CG | PHE B | | | -19.230 | 74.644 | 1.00 32.57 |
| MOTA | | | | 240 | 24.245 | 20.230 | | |
| MOTA | 4966 | CDI | PHE B | 246 | 53.548 | -20.142 | 74.989 | 1.00 27.72 |
| ATOM | 4967 | CD2 | PHE B | 246 | 54.174 | -18.048 | 74.003 | 1.00 28.20 |
| | | CEI | PHE B | 246 | | -19.878 | 74.704 | 1.00 26.71 |
| ATOM | 4968 | | FILE D | 246 | | | 73.713 | 1 00 20 27 |
| ATOM | 4969 | CE2 | PHE B | 246 | | -17.773 | | 1.00 29.27 |
| ATOM | 4970 | CZ | PHE B | 246 | 51.850 | -18.689 | 74.065 | 1.00 26.18 |
| | | | PHE B | 246 | _ | -20.040 | 72.682 | 1.00 35.32 |
| MOTA | 4971 | C | rnc D | 240 | | | | 1 00 31 73 |
| ATOM | 4972 | ၁ | PHE B | 246 | | -19.153 | 72.517 | 1.00 31.73 |
| ATOM | 4973 | 21 | GLU B | 247 | 56.205 | -20.568 | 71.683 | 1.00 37.00 |
| WI OIL | | | | | | | | |

| ATOM | 1 4974 CA GLU B 247 | 56.363 -20.137 70.296 1.00 40.73 |
|------|---------------------|--|
| ATOM | | |
| ATOM | 4989 N GLU B 249 | |
| ATOM | | |
| ATOM | 4991 CB GLU B 249 | 23.33 |
| ATOM | 4992 CG GLU B 249 | 50.374 -17.366 66.645 1.00 31.87 |
| ATOM | 4003 55 555 | 50.284 -18.867 66.787 1.00 28.64 |
| ATOM | 4994 OE1 GLU B 249 | 48.847 -19.338 66.747 1.00 33.37 |
| ATOM | 4995 OE2 GLU B 249 | 48.069 -18.917 67.630 1.00 26.38 |
| ATOM | 4996 C GLU B 249 | 48.494 -20.115 65.835 1.00 37.71 |
| ATOM | 4997 O GLU B 249 | 51.700 -15.273 66.650 1.00 28.25 |
| ATOM | 4998 N VAL B 250 | 51.776 ~14.765 65.537 1.00 21.47 |
| ATOM | 4999 CA VAL B 250 | 51.561 -14.564 67.768 1.00 21.77 |
| ATOM | 5000 CB VAL B 250 | 51.459 -13.110 67.756 1.00 21.41 |
| MOTA | 5001 CG1 VAL B 250 | 50.027 -12.676 67.357 1.00 26.42 |
| ATOM | 5002 CG2 VAL B 250 | 49.037 -13.196 68.378 1.00 20.96 |
| ATOM | 5003 C VAL B 250 | 49.931 -11.166 67.243 1.00 24.68 51.757 -12.608 69.168 1.00 22.88 |
| ATOM | 5004 O VAL B 250 | 22.00 |
| ATOM | 5005 N TYR B 251 | 50 001 |
| ATOM | 5006 CA TYR B 251 | |
| ATOM | 5007 CB TYR B 251 . | F3 0F4 |
| ATOM | 5008 CG TYR B 251 | 21.00 20.07 |
| ATOM | 5009 CD1 TYR B 251 | CC 100 |
| ATOM | 5010 CE1 TYR B 251 | 55 100 |
| MOTA | 5011 CD2 TYR B 251 | 2.00 23,75 |
| MOTA | 5012 CE2 TYR B 251 | F. F. C |
| ATOM | 5013 CZ TYR B 251 | 2.00 |
| ATOM | 5014 OH TYR B 251 | 2.00 223 |
| MOTA | 5015 C TYR B 251 | 2.00 25.10 |
| ATOM | 5016 O TYR B 251 | |
| MOTA | 5017 N LEU B 252 | 52.095 -8.622 69.728 1.00 20.14 51.834 -8.930 71.958 1.00 21.13 |
| ATOM | 5018 CA LEU B 252 | 51.533 -7.532 72.252 1.00 24.61 |
| MOTA | 5019 CB LEU B 252 | 50.154 -7.373 73.897 1.00 22.88 |
| MOTA | 5020 CG LEU B 252 | 48.915 -7.435 1.996 1.00 23.73 |
| ATOM | 5021 CD1 LEU B 252 | 48.779 -8.792 71.360 1.00 23.18 |
| MOTA | 5022 CD2 LEU B 252 | 47.697 -7.119 72.833 1.00 29.06 |
| ATOM | 5023 C LEU B 252 | 52.610 -7.044 73.217 1.00 24.77 |
| MOTA | 5024 O LEU B 252 | 53.064 -7.797 74.076 1.00 23.33 |
| MOTA | 5025 N LEU B 253 | 53.011 -5.786 73.071 1.00 20.14 |
| MOTA | 5026 CA LEU B 253 | 54.057 -5.209 73.911 1.00 20.33 |
| MOTA | 5027 CB LEU B 253 | 55.304 -4.946 73.051 1.00 15.18 |
| ATOM | 5028 CG LEU B 253 | 56.490 -4.210 73.688 1.00 18.34 |
| ATOM | 5029 CD1 LEU B 253 | 57 060 |
| MOTA | 5030 CD2 LEU B 253 | |
| MOTA | 5031 C LEU B 253 | 57.552 -3.953 72.624 1.00 19.60 53.550 -3.913 74.536 1.00 20.54 |
| ATOM | 5032 O LEU B 253 | 53.200 -2.974 73.821 1.00 22.80 |
| MOTA | 5033 N GLN B 254 | 15 405 |
| MOTA | 5034 CA GLN B 254 | 53 000 |
| MOTA | 5035 CB GLN B 254 | 53.000 -2.654 76.539 1.00 21.77 52.129 -3.040 77.755 1.00 17.85 |
| MOTA | 5036 CG GLN B 254 | 52.724 -2.815 79.124 1.00 32.51 |
| MOTA | 5037 CD GLN B 254 | 52.563 -1.396 79.609 1.00 28.19 |
| ATCM | 5038 OE1 GLN B 254 | 51.507 -0.996 80.124 1.00 26.96 |
| MOTA | 5039 NE2 GLN B 254 | 53.603 -0.619 79.432 1.00 16.80 |
| | | |

| | | | | | | | - - | |
|-------|------|-----|----------|-------|--------|--------|------------|------------|
| * mOM | 5040 | С | GLN B | 254 | 54.211 | -1.793 | 76.887 | 1.00 20.15 |
| MCTA | | | GLN B | 254 | 55.186 | 2.254 | 77.497 | 1.00 20.11 |
| MOTA | 5041 | 0 | | | | -0.532 | 76.468 | 1.00 19.46 |
| ATOM | 5042 | N. | | 255 | 54.146 | | | 1.00 15.99 |
| ATOM | 5043 | CA | LEU B | 255 | 55.268 | 0.386 | 76.614 | |
| ATOM | 5044 | CB | LEU B | 255 | 55.692 | 0.831 | 75.211 | 1.00 18.15 |
| | | CG | LEU B | | 56.143 | -0.316 | 74.296 | 1.00 21.80 |
| ATOM | 5045 | | | | 56.215 | 0.159 | 72.850 | 1.00 16.70 |
| MCTA | 5046 | | LEU B | | | -0.843 | 74.771 | 1.00 13.76 |
| ATOM | 5047 | CD2 | | 255 | 57.501 | | | |
| ATOM | 5048 | С | LEU B | 255 | 55.083 | 1.614 | 77.492 | 1.00 21.41 |
| | 5049 | | | 255 | 55.379 | 2.741 | 77.065 | 1.00 18.40 |
| ATCM | | | | 256 | 54.618 | 1.408 | 78.718 | 1.00 16.80 |
| ATOM | 5050 | N | | | | 2.519 | 79.634 | 1.00 19.90 |
| ATOM | 5051 | CA | | 256 | 54.456 | | 79.818 | 1.00 17.68 |
| ATOM | 5052 | С | | 256 · | 55.816 | 3.181 | | |
| ATOM | 5053 | 0 | GLY B | 256 | 56.854 | 2.514 | 79.841 | 1.00 13.96 |
| | 5054 | N | THR B | | 55.824 | 4.497 | 79.936 | 1.00 19.55 |
| MOTA | | | THR B | 257 | 57.081 | 5.205 | 80.098 | 1.00 19.47 |
| MOTA | 5055 | CA | | | 57.044 | 6.547 | 79.340 | 1.00 21.49 |
| MOTA | 5056 | CB | THR B | 25/ | | | 79.858 | 1.00 17.43 |
| MOTA | 5057 | OG1 | | 257 | 55.989 | 7.365 | | 1.00 22.49 |
| ATOM | 5058 | CG2 | THR B | 257 | 56.780 | 6.311 | 77.850 | |
| | 5059 | С | THR B | 257 | 57.440 | 5.466 | 81.564 | 1.00 20.75 |
| ATOM | | ō | THR B | | 58.480 | 5.054 | 81.843 | 1.00 25.01 |
| MOTA | 5060 | | | | 56.618 | 5.004 | 82.504 | 1.00 17.23 |
| Mota | 5061 | N | ASP B | | | 5.277 | 83.906 | 1.00 17.42 |
| ATOM | 5062 | CA | ASP B | 258 | 56.929 | | | 1.00 12.75 |
| ATOM | 5063 | CB | ASP B | | 55.744 | 4.940 | 84.846 | |
| ATOM | 5064 | CG | ASP B | 258 | 55.197 | 3.524 | 84.676 | 1.00 21.60 |
| | 5065 | C | ASP B | 258 | 58.245 | 4.718 | 84.460 | 1.00 16.09 |
| MOTA | 5066 | ŏ | ASP B | 258 | 58.667 | 5.116 | 85.542 | 1.00 22.07 |
| ATOM | | | | 258 | 55.901 | 2.642 | 84.150 | 1.00 17.74 |
| MOTA | 5067 | ODI | | | 54.041 | 3.281 | 85.109 | 1.00 18.68 |
| ATOM | 5068 | OD2 | ASP B | 258 | | 3.746 | 83.779 | 1.00 20.98 |
| ATOM | 5069 | N | PRO B | | 58.879 | | | 1.00 17.75 |
| MOTA | 5070 | CD | PRO B | 259 | 58.474 | 2.901 | 82.641 | |
| ATOM | 5071 | CA | PRO B | 259 | 60.154 | 3.257 | 84.321 | 1.00 22.63 |
| | 5072 | CB | PRO B | | 60.395 | 1.988 | 83.506 | 1.00 23.46 |
| ATOM | | CG | PRO B | | 59.800 | 2:343 | 82.199 | 1.00 27.08 |
| MOTA | 5073 | | PRO B | 250 | 61.305 | 4.284 | 84.172 | 1.00 23.86 |
| MOTA | 5074 | С | PRO B | 223 | 62.406 | 4.082 | 84.698 | 1.00 24.24 |
| ATOM | 5075 | 0 | PRO B | 233 | 62.400 | 5.387 | 83.465 | 1.00 20.49 |
| ATOM | 5076 | N | LEU B | 260 | 61.054 | | 83.262 | 1.00 15.17 |
| MOTA | 5077 | CA | LEU B | 260 | 62.080 | 6.417 | | 1.00 17.03 |
| ATOM | 5078 | CB | LEU B | 260 | 61.626 | 7.408 | 82.185 | |
| ATOM | 5079 | CG | LEU B | | 61.431 | 6.881 | 80.760 | 1.00 16.02 |
| | 5080 | | LEU B | | 60.703 | 7.915 | 79.901 | 1.00 17.03 |
| ATOM | | CD3 | LEU B | 260 | 62.803 | 6.546 | 80.163 | 1.00 18.58 |
| atom | 5081 | | 150 5 | 260 | 62.449 | 7.194 | 84.541 | 1.00 22.45 |
| ATOM | 5082 | С | LEU B | | | 7.440 | 85.412 | 1.00 17.84 |
| ATOM | 5083 | 0 | LEU B | | 61.611 | | 84.635 | 1.00 22.90 |
| ATOM | 5084 | N | LEU B | 261 | 63.713 | 7.588 | | 1.00 26.34 |
| ATOM | 3085 | CA | LEU B | 261 | 64.219 | 8.332 | 85.782 | |
| | 3086 | CB | LEU B | 261 | 65.605 | 8.914 | 85.473 | 1.00 20.58 |
| ATOM | | CG | | 261 | 66.180 | 9.850 | 86.553 | 1.00 28.44 |
| atom | 3087 | | | 261 | 66.481 | 9.055 | 87.812 | 1.00 29.84 |
| ATOM | 5088 | CDI | | | | 10.522 | 86.057 | 1.00 32.10 |
| ATOM | 5089 | CD2 | | 261 | 67.462 | | | 1.00 27.61 |
| ATOM | 5090 | С | LEU B | 261 | 63.315 | 9.475 | 86.227 | |
| ATOM | 5091 | 0 | LEU B | 261 | 62.978 | 9.586 | 87.408 | 1.00 24.02 |
| | 5092 | N | GLU B | | 62.934 | 10.315 | 85.269 | 1.00 23.33 |
| ATOM | | | GLU B | | 62.126 | 11.490 | 85.530 | 1.00 23.38 |
| ATOM | 5093 | CA | GLU B | 202 | 62.115 | 12.415 | 84.302 | 1.00 23.17 |
| MOTA | 5094 | CB | GLU B | 202 | | 12.854 | 83.806 | 1.00 28.98 |
| ATOM | 5095 | CG | GLU B | | 63.503 | | | 1.00 32.26 |
| ATOM | 5096 | CD | GLU B | | 64.179 | 11.831 | 82.902 | 1.00 29.28 |
| ATOM | 5097 | CE1 | GLU B | 262 | 63.702 | 10.673 | 82.838 | 1.00 29.20 |
| | 5098 | | GLU B | | 65.201 | 12.186 | 82.264 | 1.00 25.42 |
| ATOM | | C | GLU B | | 60.693 | 11.249 | 85.976 | 1.00 23.25 |
| HOTE | 5099 | | GLU B | 262 | 60.013 | 12.192 | 86.368 | 1.00 27.63 |
| ATCM | 5100 | 0 | | | | 10.011 | 85.927 | 1.00 22.25 |
| ATOM | 5101 | N | ASP B | | 60.219 | 9.751 | 86.345 | 1.00 24.46 |
| ATOM | 5102 | CA | ASP B | | 58.840 | | | |
| ATOM | 5103 | CB | ASP B | 263 | 58.214 | 8.659 | 85.465 | |
| ATOM | 5104 | CG | ASP B | | 56.710 | 8.543 | 85.659 | |
| | 5105 | | ASP B | | 55.995 | 8.318 | 84.656 | 1.00 21.82 |
| ATOM: | 3707 | | - | | . – | | • | |

| ATOM | 510 | 6 0 | D2 ASP B 2 | 53 | 56.239 | 8.66 | 86.811 | 1.00 18.31 |
|--------------|--------------|----------|------------------------|----|------------------|----------------|------------------|--------------------------|
| MOTA | 510 | 7 C | ASP B 2 | 53 | 58.834 | 9.339 | | |
| MOTA | 510 | 8 0 | ASP B 26 | 53 | 59.437 | 8.33 | | |
| ATOM | 5109 | 9 N | TYR B 26 | 4 | 58.155 | | | |
| ATOM | 5110 |) C | A TYR B 26 | 4 | 58.101 | | | |
| MOTA | 5111 | L C | B TYR B 26 | 4 | 57.511 | | | |
| MOTA | 5112 | 2 C | G TYR B 26 | 4 | 58.241 | | | |
| ATOM | 5113 | 3 C | D1 TYR B 26 | | 57.981 | | | |
| MOTA | 5114 | 1 C | E1 TYR B 26 | 4 | 58.654 | 14.370 | | |
| ATOM | 5115 | C C | D2 TYR B 26 | 4 | 59.197 | 12.779 | | |
| ATOM | 5116 | C | E2 TYR B 26 | 4 | 59.876 | 13.977 | | |
| MOTA | 5117 | C | TYR B 26 | 4 | 59.600 | 14.769 | | |
| ATOM | 5118 | 01 | TYR B 26 | 4 | 60.268 | 15.961 | | 1.00 49.65 |
| MOTA | 5119 | C | TYR B 26 | 4 | 57.340 | 8.628 | | |
| MOTA | 5120 | 0 | TYR B 26 | 4 | 57.514 | 8.181 | | |
| MOTA | 5121 | N | LEU B 26 | 5 | 56.491 | 8.074 | | |
| MOTA | 5122 | C. | LEU B 26 | 5 | 55.744 | 6.900 | | |
| ATOM | 5123 | CE | | 5 | 54.371 | 6.838 | | |
| ATOM | 5124 | CC | | | 53.415 | 7.982 | | 1.00 26.00 |
| MOTA | 5125 | CI | | | 51.970 | 7.583 | | 1.00 22.21 |
| ATOM | 5126 | CI | | | 53.530 | 8.281 | | 1.00 29.31 |
| MOTA | 5127 | C | LEU B 26 | | 56.478 | 5.568 | 89.948 | 1.00 25.83 |
| MOTA | 5128 | 0 | LEU B 26 | | 55.848 | 4.512 | 89.908 | 1.00 21.74 |
| MOTA | 5129 | N | SER B 26 | | 57.808 | 5.618 | 89.867 | 1.00 23.30 |
| ATOM | 5130 | CA | | | 58.608 | 4.398 | 89.813 | 1.00 20.75 |
| ATOM | 5131 | CB | | | 58.820 | 3.900 | 88.378 | 1.00 19.67 |
| MOTA | 5132 | OG | | | 59.863 | 4.615 | 87.739 | 1.00 18.11 |
| ATOM | 5133 | C | SER B 266 | | 59.963 | 4.710 | 90.420 | 1.00 23.01 |
| MOTA MOTA | 5134 | 0 | SER B 266 | | 60.437 | 5.845 | 90.345 | 1.00 17.74 |
| ATOM | 5135 5136 | N | LYS B 267 | | 60.590 | 3.707 | 91.023 | 1.00 24.25 |
| ATOM | 5137 | CA CB | LYS B 267 | | 61.905 | 3.916 | 91.613 | 1.00 23.79 |
| MOTA | 5138 | CG | LYS B 267 | | 62.027 | 3.153 | 92.929 | 1.00 23.71 |
| ATOM | 5139 | CD | LYS B 267 | | 60.989 | 3.582 | 93.960 | 1.00 27.29 |
| ATOM | 5140 | CE | LYS B 267 | | 61.059 | 5.088 | 94.207 | 1.00 30.33 |
| ATOM | 5141 | NZ | LYS B 267 | | 60.067 | 5.535 | 95.273 | 1.00 30.90 |
| ATOM | 5142 | c | LYS B 267 | | 60.155 62.990 | 7.004 3.483 | 95.509 | 1.00 33.37 |
| ATOM | 5143 | ō | LYS B 267 | | 64.153 | 3.403 | 90.634 91.016 | 1.00 26.41 |
| ATOM | 5144 | N | PHE B 268 | | 62.595 | 3.288 | 89.375 | 1.00 25.33 1.00 22.18 |
| MOTA | 5145 | CA | PHE B 268 | | 63.529 | 2.919 | 88.318 | 1.00 22.18 |
| ATOM | 5146 | CB | PHE B 268 | | 62.814 | 2.171 | 87.179 | 1.00 20.55 |
| ATOM | 5147 | CG | PHE B 268 | | 62.389 | 0.761 | 87.526 | 1.00 19.23 |
| MOTA | 5148 | CDI | PHE B 268 | | 61.722 | -0.025 | 86.585 | 1.00 20.72 |
| MOTA | 5149 | CD2 | PHE B 268 | | 62.673 | 0.207 | 88.773 | 1.00 18.17 |
| ATOM | 5150 | CE1 | PHE B 268 | | 61.344 | -1.336 | 86.875 | 1.00 18.83 |
| ATOM | 5151 | CE2 | | | 62.300 | -1.105 | 89.073 | 1.00 20.05 |
| MOTA | 5152 | CZ | PHE B 268 | | 61.634 | -1.879 | 88.122 | 1.0' 19.70 |
| ATOM | 5153 | С | PHE B 268 | | 64.114 | 4.222 | 87.785 | 1.01 23.66 |
| ATOM | 5154 | 0 | PHE B 268 | | 63.412 | 5.232 | 87.692 | 1.00 19.40 |
| ATOM | 5155 | N | ASN B 269 | | 65.396 | 4.203 | 87.437 | 1.00 21.96 |
| ATOM | 5156 | CA | ASN B 269 | | 66.060 | 5.396 | 86.926 | 1.00 25.04 |
| ATOM | 5157 | CB | ASN B 269 | | 67.243 | 5.783 | 87.824 | 1.00 25.68 |
| ATOM | 5158 | CG | ASN B 269 | | 66.845 | 5.946 | 89.273 | 1.00 27.04 |
| MOTA | 5159 | | ASN B 269 | | 65.832 | 6.557 | 89.579 | 1.00 28.81 |
| MOTA MOTA | 5160 | | ASN B 269 | | 67.659 | 5.419 | 90.176 | 1.00 31.12 |
| | 5161 | C | ASN B 269 | | 66.579 | 5.151 | 85.523 | 1.00 25.87 |
| ATOM | 5162 5163 | O N | ASN B 269 | | 67.769 | 5.336 | 85.268 | 1.00 24.58 |
| MOTA MOTA | | N CA | LEU B 270 | | 65.695 | 4.757 | 84.611 | 1.00 21.37 |
| atom atom | | CB | LEU B 270 LEU B 270 | | 66.116 | 4.462 | 83.241 | 1.00 16.35 |
| ATOM ATOM | | CG | LEU B 270 | | 65.176 64.909 | 3.426 | 82.610 | 1.00 24.12 |
| ATOM | | | LEU B 270 | | | 2.144 | 83.412 | 1.00 27.89 |
| ATOM | 5168 | CD2 | LEU B 270 | | 64.181 66.221 | 1.136 | 82.515 | 1.00 -23.01 |
| ATOM | | CD2 | LEU B 270 | | 66.184 | 1.547 | 83.904 | 1.00 23.92 |
| MOTA | | ō | LEU B 270 | | 65.654 | 5.682 6.761 | 82.337 82.663 | 1.00 20.06 |
| ATOM | | N | SER B 271 | | 66.839 | 5.497 | 81.193 | 1.00 16.34 |
| • | _ | - | | | | J.431 | - | 1.00 20.07 |

Figure 18-79

| ATOM | 3637 | | | | | | - | |
|--------------|--------------|----------|------------------------|---|------------------|------------------|------------------|--------------------------|
| ATOM | 5236 5237 | CE: | 2 PHE B 279 | | 60.001 | -0.051 | | 1.00 25.57 |
| MOTA | 5235 | CD | 2 PHE B 279 | | 58.325 | -1.162 | 69.799 | |
| MOTA | 5234 | CD. | 2 PHE B 279 | | 60.862 | -0.078 | 69.567 | |
| ATOM | 5233 | CG | 1 PHE B 279 | | 59.196 | -1.182 | 70.882 | |
| ATOM | 5232 | CB | PHE B 279 | | 60.467 | -0.640 | 70.778 | |
| MOTA | 5231 | CA | PHE B 279 | | 61.395 | -0.629 | 71.955 | |
| ATOM | 5230 | N | PHE B 279 | | 61.860 | -2.014 | 72.398 | 1.00 22.74 |
| MOTA | 5229 | 0 | ALA B 278 PHE B 279 | | 62.849 | -1.862 | 73.464 | 1.00 24.79 |
| ATOM | 5228 | C | ALA B 278 | | 63.231 | -4.068 | | 1.00 19.27 |
| ATOM | 5227 | CB | ALA B 278 | | 63.752 | -2.896 | | 1.00 22.68 |
| ATOM | 5226 | CA | ALA B 278 | | 64.476 63.752 | -2.117 | | 1.00 17.34 |
| ATOM | 5225 | 11 | ALA B 278 | | 65.319 | -2.544 | 75.114 | |
| ATOM | 5224 | 0 | LYS B 277 | | 65.987 | -2.568 -1.454 | 74.624 | 1.00 22.32 |
| MOTA | 5223 | С | LYS B 277 | | 66.000 | -1.554 | 72.777 | 1.00 19.90 |
| MOTA | 5222 | NZ | LYS B 277 | | 70.616 | -2.586 1.554 | 71.230 73.482 | 1.00 24.22 |
| ATOM | 5221 | CE | LYS B 277 | | 70.283 | -3.137 | 72.580 | 1.00 44.67 |
| ATOM | 5220 | CD | LYS B 277 | | 69.061 | -2.456 | | |
| ATOM | 5219 | CG | LYS 3 277 | | 69.303 | -0.973 | 73.381 73.188 | 1.00 43.87 |
| ATOM | 5218 | CB | LYS B 277 | | 68.086 | -0.239 | 73.938 | 1.00 27.57 |
| ATOM | 5217 | CA | LYS 3 277 | | 66.823 | -0.335 | | 1.00 27.37 |
| ATOM | 5216 | N | LYS B 277 | | 66.011 | 0.857 | 73.261 73.076 | 1.00 24.36 |
| ATOM | 5215 | õ | LEU B 276 | | 64.348 | 0.191 | 71.886 | 1.00 20.73 |
| MOTA MOTA | 5214 | č | LEU B 276 | | 64.841 | 1.021 | 72.653 | 1.00 22.33 |
| ATOM | 5213 | CD2 | LEU B 276 | | 65.840 | 4.312 | 70.018 | 1.00 21.01 |
| ATOM | 5211 | נתם | LEU B 276 | | 63.818 | 2.852 | 69.936 | 1.00 24.81 1.00 21.01 |
| MOTA | 5210 | CG | LEU B 276 | | 65.114 | 3.132 | 70.662 | 1.00 24.94 |
| ATOM | 5209 5210 | CA CB | LEU B 276 | | 64.814 | 3.421 | 72.134 | 1.00 19.87 |
| ATOM | 5208 | N CA | LEU B 276 | | 64.128 | 2.330 | 72.946 | 1.00 21.28 |
| MOTA | 5207 | O N | LEU B 276 | | 64.183 | 2.648 | 74.378 | 1.00 23.85 |
| ATOM | 5206 | С | PHE B 275 | | 63.045 | 0.821 | 75.030 | 1.00 22.68 |
| ATOM | 5205 | CZ | PHE B 275 | | 63.642 | 1.860 | 75.305 | 1.00 24.47 |
| MOTA | 5204 | CE2 | PHE B 275 | | 58.727 | 2.851 | 76.701 | 1.00 25.78 |
| MOTA | 5203 | | | | 59.365 | 3.670 | 75.795 | 1.00 27.62 |
| MOTA | 5202 | CD2 | PHE B 275 | | 59.450 | 2.254 | 77.722 | 1.00 27.82 |
| ATOM · | 5201 | CDI | PHE B 275 | | 60.732 | 3.893 | 75.907 | 1.00 27.31 |
| MOTA | 5200 | CG | PHE B 275 PHE B 275 | | 60.815 | 2.483 | 77.826 | 1.00 23.64 |
| MOTA | 5199 | CB | | | 61.466 | 3.303 | 76.921 | 1.00 24.72 |
| ATOM | 5198 | CA | PHE B 275 | | . 62.941 | 3.546 | 77.637 | 1.00 22.24 |
| ATOM | 5197 | N | PHE B 275 | | 63.802 | 2.310 | 76.761 | 1.00 21.25 |
| ATOM | 5196 | 0 N | PHE B 275 | | 65.207 | 2.631 | 77.003 | 1.00 18.50 |
| MOTA | 5195 | C | ALA B 274 | | 65.962 | 0.567 | 76.525 | 1.00 20.77 |
| MOTA | 5194 | CB | ALA B 274 | | 66.172 | 1.729 | 76.863 | 1.00 18.23 |
| MOTA | 5193 | CA | ALA B 274 | | 67.858 | 2.195 | 78.646 | 1.00 19.09 |
| ATOM | 5192. | N | ALA B 274 | | 67.589 | 2.220 | 77.151 | 1.00 18.12 |
| MOTA | 5191 | 0 | ALA B 274 | | 67.690 | 3.580 | 76.648 | 1.00 20.96 |
| ATOM | 5190 | C | VAL B 273 VAL B 273 | ٠ | 67.590 | 2.913 | 74.513 | 1.00 24.19 |
| MOTA | 5189 | | VAL B 273 | | 67.664 | 3.812 | 75.343 | 1.00 24.23 |
| MOTA | 5188 | . CG1 | VAL B 273 | | 69.299 | 7.057 | 74.115 | 1.00 33.57 |
| ATOM | 5187 | CB | VAL B 273 | | 70.036 | 4.691 | 74.029 | 1.00 34.98 |
| ATOM | 5186 | CA | VAL B 273 | | 67.745 69.225 | 5.705 | 74.805 | 1.00 30.40 |
| MOTA | 5185 | N | VAL B 273 | | 67.012 | 5.260 | 74.899 | 1.00 27.34 |
| ATOM | 5184 | 0 | ASN B 272 | | 64.967 | 5.280 6.160 | 75.774 | 1.00 20.40 |
| ATOM | 5183 | С | ASN B 272 | | 65.701 | 6.088 5.280 | 75.412 | 1.00 23.12 |
| ATOM | 5182 | ND2 | ASN B 272 | | 63.299 | 9.052 | 75.974 | 1.00 26.88 |
| ATOM | 5181 | OD1 | ASN B 272 | | 64.167 | 10.575 | 77.360 | 1.00 41.69 |
| MOTA | 5180 | CG. | ASN B 272 | | 64.198 | 9.456 | 75.946 | 1.00 37.72 |
| ATOM | 5179 | CB | ASN B 272 | | 65.263 | 8.478 | 76.123 | 1.00 37.83 |
| ATOM | 5178 | CA | ASN B 272 | | 65.152 | 7.156 | 76.906 76.123 | 1.00 30.30 |
| MOTA | 5177 | N | ASN B 272 | | 65.916 | 7.238 | 78.154 | 1.00 20.84 |
| MOTA MOTA | 5176 | õ | SER B 271 | | 65.631 | 5.102 | 78.854 | 1.00 16.12 1.00 20.84 |
| ATOM | 5175 | C | SER B 271 | | 66.106 | 6.228 | 79.000 | 1.00 22.83 |
| ATOM | 5174 | OG | SER B 271 | | 68.772 | 5.485 | 78.921 | 1.00 21.47 |
| MOTA | 5173 | CB | SER B 271 | | 68.437 | 6.621 | 79.714 | 1.00 21.80 |
| | 5172 | CA | SER B 271 | | 66.989 | 6.546 | 80.200 | 1.00 21.20 |
| | | | | | | | | |

| ATOM | 5238 | CZ | PHE | B 279 | 58.72 | 7 -0.594 | 68.592 | 1.00 25.13 |
|--------|------|-----|-------|-------|---------|----------|---------|------------|
| ATOM | 5239 | c | | B 279 | 62.47 | | 71.212 | 1.00 23.60 |
| ATOM | 5240 | ō | | B 279 | 61.86 | | 70.678 | 1.00 26.54 |
| | 5241 | N | | B 280 | 63.67 | | 70.804 | 1.00 21.93 |
| ATOM | 5242 | CA | | B 280 | 64.31 | | 69.680 | |
| MOTA | | | | | | | | 1.00 23.70 |
| MOTA | 5243 | CB | | B 280 | 65.52 | | 69.164 | 1.00 22.63 |
| 'ATOM | 5244 | CG | | B 280 | 65.10 | | 68.505 | 1.00 30.83 |
| MOTA | 5245 | OD: | | B 280 | 64.09 | | 67.796 | 1.00 25.81 |
| MOTA | 5246 | ND | | B-280 | 65.90 | | 68.714 | 1.00 26.54 |
| ATOM | 5247 | С | ASN I | B 280 | 64.74 | | 70.009 | 1.00 26.10 |
| MOTA | 5248 | 0 | ASN 1 | B 280 | - 64.77 | 5 -5.321 | 69.124 | 1.00 26.16 |
| MOTA | 5249 | N | ILE ! | B 281 | 65.08 | 0 -4.724 | 71.272 | 1.00 26.10 |
| MOTA | 5250 | CA | ILE 1 | 3 281 | 65.48 | 5 -6.067 | 71.667 | 1.00 25.81 |
| ATOM | 5251 | CB | ILE I | 3 281 | 66.00 | 5 -6.098 | 73.124 | 1.00 28.50 |
| ATOM | 5252 | CG2 | ILE 1 | 3 281 | 66.04 | 6 -7.527 | 73.648 | 1.00 28.53 |
| ATOM | 5253 | CG1 | ILE I | 3 281 | 67.39 | 2 -5.454 | 73.173 | 1.00 32.07 |
| MOTA | 5254 | CDI | ILE I | 3 281 | . 68.03 | 3 -5.442 | 74.541 | 1.00 28.24 |
| MOTA | 5255 | С | ILE I | 3 281 | 64.32 | 7.030 | 71.507 | 1.00 25.77 |
| ATOM | 5256 | 0 | ILE E | 3 281 | 64.48 | 4 -8.131 | 70.982 | 1.00 23.39 |
| ATOM | 5257 | N | VAL I | 3 282 | 63.13 | | 71.950 | 1.00 21.30 |
| ATOM | 5258 | CA | VAL I | | 61.96 | | 71.813 | 1.00 22.90 |
| ATOM | 5259 | CB | VAL I | | 60.70 | | 72.387 | 1.00 24.07 |
| ATOM | 5260 | | VAL E | | 59.46 | | 72.093 | 1.00 22.28 |
| ATOM | 5261 | CG2 | | | 60.86 | | 73.906 | 1.00 26.89 |
| ATOM | 5262 | c | VAL E | | 61.71 | | 70.339 | 1.00 23.87 |
| ATOM | 5263 | ō | VAL | | 61.462 | | 69.978 | 1.00 22.65 |
| ATOM | 5264 | N | ARG E | | 61.799 | | 69.488 | 1.00 23.19 |
| ATOM | 5265 | CA | ARG E | | 61.57 | | 68.060 | 1.00 27.95 |
| ATOM | 5266 | СВ | ARG E | | 61.510 | | 67.359 | 1.00 25.48 |
| ATOM | 5267 | CG | ARG E | | 60.33 | | 67.838 | 1.00 26.55 |
| ATOM | 5268 | CD | ARG E | | 60.442 | | 67.339 | 1.00 31.52 |
| ATOM | 5269 | NE | ARG E | | 60.210 | | 65.908 | 1.00 24.43 |
| ATOM | 5270 | CZ | ARG E | | 60.919 | | 65.116 | 1.00 26.45 |
| ATOM | 5271 | | | | 61.902 | | 65.622 | 1.00 26.04 |
| ATOM | 5272 | NH2 | | | 60.634 | | 63.825 | 1.00 29.64 |
| ATOM | 5273 | С | ARG E | | 62.634 | | 67.402 | 1.00 32.04 |
| ATOM | 5274 | Ō | ARG E | | 62.341 | | 66.431 | 1.00 29.76 |
| MOTA | 5275 | N | GLU B | | 63.859 | | 67.923 | 1.00 31.50 |
| ATOM | 5276 | CA | GLU B | 284 | 64.934 | -8.646 | 67.381 | 1.00 32.42 |
| ATOM | 5277 | CB | GLU B | 284 | 66.289 | -8.260 | 67.992 | 1.00 38.31 |
| ATOM | 5278 | CG | GLU B | 284 | 66.798 | -6.864 | 67.640 | 1.00 48.93 |
| MOTA | 5279 | CD | GLU B | 284 | 68.102 | -6.518 | 68.362 | 1.00 56.28 |
| MOTA | 5280 | OE1 | GLU B | 284 | 69.084 | -7.281 | 68.222 | 1.00 57.37 |
| MOTA | 5281 | OE2 | GLU B | 284 | 68.150 | -5.485 | 69.069 | 1.00 55.42 |
| MOTA . | 5282 | С | GLU B | 284 | 64.638 | -10.105 | 67.714 | 1.00 31.93 |
| ATOM | 5283 | 0 | GLU B | 284 | 64.899 | -11.001 | 66.913 | 1.00 28.26 |
| MOTA | 5284 | N | VAL B | 285 | 64.089 | -10.340 | 68.901 | 1.00 28.09 |
| MOTA | 5285 | CA | VAL B | | 63.765 | -11.697 | 69.325 | 1.00 30.67 |
| ATOM | 5286 | CB | VAL B | | | -11.802 | 70.863 | 1.00 28.33 |
| ATOM | 5287 | CGl | VAL B | 285 | 63.257 | -13.206 | 71.262 | 1.00 29.84 |
| ATOM | 5288 | CG2 | VAL B | | | -11.470 | 71.478 | 1.00 26.93 |
| MOTA | 5289 | С | VAL B | 285 | | -12.265 | 68.758 | 1.00 31.19 |
| ATOM | 5290 | 0 | VAL B | | 62.422 | -13.423 | 68.349 | 1.00 31.38 |
| ATOM | 5291 | N | PHE B | | 61.398 | -11.460 | 68.729 | 1.00 28.21 |
| MOTA | 5292 | CA | PHE B | 286 | | -11.948 | 68.249 | 1.00 25.71 |
| ATOM | 5293 | CB | PHE B | 286 | | -11.853 | 69.374 | 1.00 24.57 |
| ATOM | 5294 | CG | PHE B | 286 | 59.311 | -12.804 | 70.514 | 1.00 26.87 |
| ATOM | 5295 | CD1 | PHE B | | | -12.331 | 71.779 | 1.00 25.16 |
| ATOM | 5296 | CD2 | PHE B | | | -14.180 | 70.319 | 1.00 22.51 |
| ATOM: | 5297 | CEl | PHE B | | | -13.213 | 72.833 | 1.00 22.92 |
| ATOH | 5298 | CE2 | PHE 3 | | | -15.063 | 71.362 | 1.00 21.99 |
| ATOM | 5299 | CZ | PHE 2 | | | -14.578 | 72.626 | 1.00 26.75 |
| ATOM | 5300 | C | PHE B | 286 | | -11.318 | 66.993 | 1.00 25.90 |
| ATOM- | 5301 | 0 | PHE B | 286 | _ | -11.630 | 66.620 | 1.00 22.84 |
| MOTA | 5302 | N | GLY B | 287 | 60.272 | | 66.329 | 1.00 28.27 |
| ATON | 5303 | CA | GLY B | 287 | 59.756 | -9.814 | .65.130 | 1.00 23.38 |
| - | | | | | | | | |

| ATOM 5310 CD GLU B 288 57.906 -4.769 63.347 1.00 41.14 ATOM 5311 OE1 GLU B 288 57.058 -4.055 63.919 1.00 41.16 ATOM 5312 OE2 GLU B 288 55.068 -4.055 63.919 1.00 41.16 ATOM 5313 C GLU B 288 55.682 -7.819 65.527 1.00 27.8 ATOM 5314 O GLU B 288 55.682 -7.819 65.527 1.00 27.8 ATOM 5315 N GLY B 289 55.176 -6.973 66.439 1.00 24.5 ATOM 5316 CA GLY B 289 55.176 -6.973 66.439 1.00 24.5 ATOM 5317 C GLY B 289 53.015 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.9 ATOM 5320 CA VAL B 290 52.171 -6.142 68.268 1.00 23.9 ATOM 5321 CB VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5323 CG2 VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5324 C VAL B 290 49.794 -5.655 69.047 1.00 22.2 ATOM 5325 O VAL B 290 51.722 -4.232 69.593 1.00 21.3 ATOM 5326 N TYR B 291 51.960 -4.741 70.687 1.00 21.3 ATOM 5327 CA TYR B 291 51.994 -6.744 70.687 1.00 21.3 ATOM 5328 CB TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5330 CD1 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5333 CZ2 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5333 CZ2 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5334 CZ TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5335 CD TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5337 CA LEU B 292 49.765 -1.369 74.411 1.00 21.7 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5340 C LEU B 292 49.765 -1.360 74.411 1.00 21.7 ATOM 5340 C B LEU B 292 55.540 9.77 9.14 1.00 22.7 ATOM 5340 C B LEU B 292 55.540 9.77 9.79 14 1.00 22.9 ATOM 5341 C G LEU B 292 55.540 9.77 9.79 14 1.00 22.9 ATOM 5340 C B LEU B 292 55.540 9.77 9.99 16 1.00 19.5 ATOM 5340 C B LEU B 292 55.540 9.77 9.99 16 1.00 19.5 ATOM 5340 C B LEU B 292 55.514 9.78 9.79 9.91 1.00 22.5 ATOM 5340 C B LEU B 292 55.514 9.80 9.80 9.80 9.80 1.00 20.7 ATOM 5340 C B LEU B 292 55.514 9.80 9.80 9 | | | | | | | | | | |
|--|-------|------|-----|---------|-----|---|---------|--------|--------|------------|
| ATCH 5306 O GLY B 287 | | E204 | ~ | CT 17 D | 207 | | 58 765 | -8 719 | 65 498 | 1.00 29.17 |
| ATOM 5306 N GLU B 288 57.896 -8.361 64.558 1.00 26.77 ATOM 5307 CA GLU B 288 55.893 -7.324 64.754 1.00 25.37 ATOM 5308 CB GLU B 288 56.405 -6.791 63.405 1.00 29.57 ATOM 5310 CD GLU B 288 57.430 -6.030 62.605 1.00 36.0 ATOM 5311 OEL GLU B 288 57.430 -6.033 62.605 1.00 36.0 ATOM 5312 OEZ GLU B 288 57.058 -4.503 63.347 1.00 41.11 ATOM 5313 C GLU B 288 57.058 -4.055 63.347 1.00 41.11 ATOM 5313 C GLU B 288 57.058 -4.055 63.347 1.00 44.67 ATOM 5313 C GLU B 288 57.058 -4.053 63.348 1.00 24.57 ATOM 5314 O GLU B 288 55.602 -7.819 65.527 1.00 27.88 ATOM 5315 N GLY B 289 55.076 -6.973 66.419 1.00 24.57 ATOM 5316 CA GLY B 289 55.076 -6.973 66.419 1.00 24.57 ATOM 5316 CA GLY B 289 55.076 -6.973 66.419 1.00 24.57 ATOM 5317 C GLY B 289 53.005 -5.326 66.358 1.00 26.17 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.17 ATOM 5319 N VAL B 290 51.194 -5.079 68.440 1.00 23.9 ATOM 5321 CE VAL B 290 51.194 -5.079 68.440 1.00 23.9 ATOM 5322 CGL VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5323 CGL VAL B 290 49.794 -5.655 69.047 1.00 18.7 ATOM 5323 CGL VAL B 290 51.960 -4.741 70.687 1.00 19.2 ATOM 5323 CGL VAL B 290 51.960 -4.741 70.687 1.00 19.2 ATOM 5323 CGL VAL B 290 51.960 -4.741 70.687 1.00 22.3 ATOM 5323 CGL VAL B 290 51.960 -4.741 70.687 1.00 22.3 ATOM 5325 O VAL B 290 51.960 -4.741 70.687 1.00 22.0 ATOM 5327 CA TYR B 291 53.522 -2.023 69.533 1.00 21.5 ATOM 5331 CB TYR B 291 55.500 -2.712 66.809 1.00 21.3 ATOM 5332 CGL VAL B 290 51.960 -4.741 70.687 1.00 22.0 ATOM 5333 CB TYR B 291 55.550 -2.712 66.809 1.00 21.3 ATOM 5333 CB TYR B 291 55.550 -2.712 66.809 1.00 21.3 ATOM 5334 C TYR B 291 55.550 -2.712 66.809 1.00 20.2 ATOM 5335 CH TYR B 291 55.550 -2.712 66.809 1.00 20.2 ATOM 5336 C TYR B 291 55.550 -2.712 66.809 1.00 20.0 ATOM 5337 CA TYR B 291 55.550 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.550 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.550 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.550 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.550 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.550 -2.712 66.809 | | | | | | | | | | |
| ATOM 5306 N GLU B 288 55.993 -7.324 64.754 1.00 25.7 ATOM 5308 CB GLU B 288 56.405 -6.791 63.405 1.00 25.5 ATOM 5308 CB GLU B 288 57.906 -4.769 63.347 1.00 41.11 ATOM 5310 CD GLU B 288 57.906 -4.769 63.347 1.00 41.11 ATOM 5310 CD GLU B 288 57.906 -4.769 63.347 1.00 41.11 ATOM 5311 OEL GLU B 288 57.906 -4.769 63.347 1.00 41.11 ATOM 5312 OEL GLU B 288 57.906 -4.769 63.347 1.00 41.11 ATOM 5313 C .06LU B 288 55.209 -4.503 63.348 1.00 44.6 ATOM 5313 C .06LU B 288 55.209 -8.911 65.527 1.00 27.8 ATOM 5314 O GLU B 288 55.209 -8.911 65.308 1.00 26.8 ATOM 5314 O GLU B 288 55.209 -8.911 65.308 1.00 26.8 ATOM 5316 CA GLY B 289 55.176 -6.973 66.419 1.00 24.5 ATOM 5316 CA GLY B 289 55.176 -6.973 66.419 1.00 29.1 ATOM 5317 C GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5319 N VAL B 290 51.194 -5.079 68.400 1.00 22.2 ATOM 5320 CA VAL B 290 51.194 -5.079 68.401 1.00 22.2 ATOM 5321 CB VAL B 290 49.794 -5.655 68.047 1.00 22.4 ATOM 5322 CG1 VAL B 290 49.794 -5.655 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 49.889 -6.504 67.629 1.00 10.2 ATOM 5323 CG2 VAL B 290 51.194 -5.079 68.401 1.00 12.2 ATOM 5325 O VAL B 290 51.950 -4.741 70.667 1.00 10.2 ATOM 5325 C VAL B 290 51.950 -4.741 70.667 1.00 12.3 ATOM 5325 C VAL B 290 51.950 -4.741 70.667 1.00 12.3 ATOM 5325 O VAL B 291 51.950 -4.741 70.667 1.00 20.3 ATOM 5325 C VAL B 291 51.950 -4.741 70.667 1.00 20.3 ATOM 5325 C VAL B 291 51.950 -4.741 70.667 1.00 20.2 ATOM 5326 N TYR B 291 51.950 -4.741 70.667 1.00 20.2 ATOM 5327 CA TYR B 291 51.950 -4.741 70.667 1.00 20.2 ATOM 5328 CB TYR B 291 51.950 -4.741 70.667 1.00 20.2 ATOM 5330 CD1 TYR B 291 51.950 -4.741 70.667 1.00 20.0 ATOM 5331 CEL TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5331 CEL TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5331 CEL TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5331 CEL TYR B 291 55.530 -4.741 70.667 71.00 22.9 ATOM 5334 C C LEU B 292 55.500 604 -7.77 71.600 71.00 20.0 ATOM 5336 C LEU B 292 55.500 604 -7.77 | ATCM | 5305 | 0 | GLY B | 287 | | 58.786 | -8.210 | | |
| ATOM 5300 CB GLU B 288 56.893 -7.324 64.754 1.00 25.34 ATOM 5300 CB GLU B 288 55.405 -6.791 63.405 1.00 29.54 ATOM 5310 CD GLU B 288 57.430 -6.003 62.605 1.00 36.00 ATOM 5311 OBI GLU B 288 57.430 -4.769 63.347 1.00 41.11 ATOM 5312 OBE GLU B 288 57.906 -4.769 63.347 1.00 41.12 ATOM 5313 C GLU B 288 57.906 -4.769 63.347 1.00 41.12 ATOM 5313 C GLU B 288 55.209 -8.931 65.527 1.00 27.8 ATOM 5314 O GLU B 288 55.209 -8.931 65.527 1.00 27.8 ATOM 5315 N GLY B 289 55.176 -6.973 66.449 1.00 24.6 ATOM 5316 CA GLY B 289 55.176 -6.973 66.449 1.00 24.1 ATOM 5316 CA GLY B 289 55.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5312 CB VAL B 290 52.171 -6.142 68.268 1.00 22.2 ATOM 5321 CB VAL B 290 49.794 -5.655 68.783 1.00 22.2 ATOM 5322 CG VAL B 290 49.794 -5.656 68.783 1.00 12.2 ATOM 5322 CG VAL B 290 49.794 -5.656 68.783 1.00 12.2 ATOM 5322 CG VAL B 290 49.794 -5.656 68.783 1.00 12.2 ATOM 5322 CG VAL B 290 49.289 -6.504 67.629 1.00 12.2 ATOM 5322 CG VAL B 290 51.794 -75.655 69.793 1.00 12.5 ATOM 5322 CG VAL B 290 51.794 -75.655 69.793 1.00 12.5 ATOM 5322 CG VAL B 290 51.794 -75.655 69.793 1.00 12.5 ATOM 5322 CG TYR B 291 51.913 -2.941 69.346 1.00 22.0 ATOM 5326 CR TYR B 291 51.913 -2.941 69.346 1.00 22.0 ATOM 5327 CA TYR B 291 52.479 -2.063 70.357 1.00 19.5 ATOM 5323 CG2 VAL B 290 51.500 -4.741 70.687 1.00 21.5 ATOM 5323 CG2 TYR B 291 52.479 -2.063 70.357 1.00 19.5 ATOM 5323 CG2 TYR B 291 52.479 -2.063 70.357 1.00 19.5 ATOM 5333 CG2 TYR B 291 52.479 -2.063 70.357 1.00 19.5 ATOM 5333 CG2 TYR B 291 55.580 -2.772 68.918 1.00 20.4 ATOM 5335 CH TYR B 291 55.580 -2.772 68.918 1.00 20.4 ATOM 5335 CH TYR B 291 55.580 -2.772 68.918 1.00 20.9 ATOM 5335 CH TYR B 291 55.600 -4.741 70.687 71.00 19.5 ATOM 5330 CD1 TYR B 291 55.600 -4.741 70.697 71.00 20.0 20.4 ATOM 5336 CH TYR B 291 55.600 -4.741 70.697 71.00 20.0 20.4 ATOM 5336 CH TYR B 291 55.600 -4.741 70.697 70.00 20.0 20.0 ATOM 5330 CD1 TYR B | | 5306 | N | GLU B | 288 | | 57.896 | -8.361 | 64.558 | 1.00 26.77 |
| ATOM 5300 CG GLU B 288 55.405 -6.791 63.405 1.00 29.5: ATOM 5310 CD GLU B 288 57.430 -6.003 62.605 1.00 36.0 ATOM 5311 OEL GLU B 288 57.058 -4.055 63.347 1.00 41.1: ATOM 5312 OE2 GLU B 288 57.058 -4.055 63.347 1.00 41.1: ATOM 5313 C GLU B 288 57.058 -4.053 63.348 1.00 44.1: ATOM 5313 C GLU B 288 55.682 -7.819 65.527 1.00 27.8: ATOM 5314 O GLU B 288 55.682 -7.819 65.527 1.00 27.8: ATOM 5315 N GLY B 289 55.005 -6.973 66.439 1.00 24.5: ATOM 5316 CA GLY B 289 55.006 -7.326 67.204 1.00 29.1: ATOM 5317 C GLY B 289 55.005 -6.171 67.244 1.00 30.4: ATOM 5318 O GLY B 289 55.005 -6.376 66.358 1.00 26.1: ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.9: ATOM 5321 CB VAL B 290 51.94 -5.079 68.400 1.00 22.3: ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5323 CG2 VAL B 290 49.794 -5.655 69.047 1.00 22.5: ATOM 5324 C VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5325 O VAL B 290 51.994 -5.079 68.401 1.00 22.1 ATOM 5326 N TYR B 291 51.913 -2.941 69.366 1.00 22.1 ATOM 5327 CA VAL B 290 51.722 -4.232 69.531 1.00 21.3 ATOM 5328 CE TYR B 291 51.913 -2.941 69.366 1.00 22.1 ATOM 5328 CE TYR B 291 51.913 -2.941 69.366 1.00 22.1 ATOM 5329 CG TYR B 291 51.933 -2.941 69.366 1.00 22.1 ATOM 5320 COL AND B 291 51.933 -2.941 69.366 1.00 22.1 ATOM 5321 CB VAL B 291 51.933 -2.941 69.366 1.00 22.0 ATOM 5326 N TYR B 291 51.933 -2.941 69.597 1.00 12.3 ATOM 5327 CA TYR B 291 51.936 -4.741 70.687 1.00 21.3 ATOM 5328 CB TYR B 291 51.936 -4.741 70.687 1.00 21.0 ATOM 5330 CD1 TYR B 291 51.936 -2.712 66.809 1.00 21.0 ATOM 5331 CE LU B 292 51.524 -4.232 69.577 1.00 12.2 ATOM 5330 CD1 TYR B 291 55.560 -4.741 70.687 1.00 21.0 ATOM 5331 CE LU B 292 51.524 -4.232 69.577 1.00 12.2 ATOM 5330 CD2 LU B 291 55.560 -4.741 70.687 1.00 22.8 ATOM 5331 CE LU B 292 51.524 -4.232 69.577 1.00 12.3 ATOM 5330 CD2 LU B 291 55.756 0.70 -7.756 89.91 1.00 20.6 ATOM 5331 CB LU B 292 51.50 -4.741 70.687 1.00 20.0 ATOM 5330 CD2 LU B 292 51.50 -4.741 70.687 1.00 20.0 ATOM 5330 CD3 ATOM 50.00 ATOM | | | | | | | | | | |
| ATOM 5310 CD GLU B 288 57, 430 -6,003 62,605 1,00 36,00 ATOM 5311 OD1 GLU B 288 57,058 -4,055 63,347 1,00 41,11 ATOM 5312 OE2 GLU B 288 57,058 -4,055 63,919 1,00 41,11 ATOM 5312 OE2 GLU B 288 57,058 -4,053 63,488 1,00 44,66 ATOM 5313 C GLU B 288 55,209 -8,931 65,338 1,00 24,68 ATOM 5314 O GLU B 288 55,209 -8,931 65,336 1,00 26,8 ATOM 5315 N GLY B 289 55,176 -6,973 66,439 1,00 24,5 ATOM 5316 CA GLY B 289 55,176 -6,973 66,439 1,00 24,5 ATOM 5316 CA GLY B 289 55,176 -6,973 66,439 1,00 24,5 ATOM 5318 O GLY B 289 53,005 -6,171 67,244 1,00 30,4 ATOM 5318 O GLY B 289 53,005 -6,171 67,244 1,00 30,4 ATOM 5319 N VAL B 290 52,171 -6,122 68,268 1,00 22,2 ATOM 5320 CA VAL B 290 52,171 -6,162 68,268 1,00 22,2 ATOM 5321 CB VAL B 290 48,89 -6,504 67,629 1,00 19,2 ATOM 5323 CC2 VAL B 290 49,794 -5,655 68,763 1,00 18,2 ATOM 5323 CC2 VAL B 290 49,289 -6,504 67,629 1,00 19,2 ATOM 5325 O VAL B 290 51,960 -4,741 70,667 1,00 22,3 ATOM 5326 N TYR B 291 51,930 -2,941 69,346 1,00 21,3 ATOM 5327 CA TYR B 291 51,930 -2,941 69,346 1,00 21,3 ATOM 5328 CB TYR B 291 51,940 -4,741 70,667 1,00 22,3 ATOM 5328 CB TYR B 291 53,552 -1,216 69,711 1,00 20,4 ATOM 5331 CB TYR B 291 54,750 -1,741 70,667 1,00 20,6 ATOM 5331 CB TYR B 291 55,580 -2,712 66,899 1,00 19,2 ATOM 5332 CC1 VAL B 290 51,960 -4,741 70,667 1,00 20,0 ATOM 5331 CB TYR B 291 54,553 -2,072 68,918 1,00 21,3 ATOM 5332 CC TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5331 CB TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5330 CD TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5330 CD TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5330 CD TYR B 291 55,580 -2,712 66,809 1,00 20,0 ATOM 5330 CD TYR B 291 50,600 -2,712 66,918 1,00 20,0 ATOM 5330 CD TYR B 291 50,600 -2,712 66,918 1 | ATOM | 5307 | CA | | | | | | | • |
| ATOM 5310 CD GLUB 288 57.430 -6.003 62.605 1.00 36.00 ATOM 5311 OBL GLUB 288 57.058 -4.055 63.347 1.00 41.11 ATOM 5311 OBL GLUB 288 57.058 -4.055 63.349 1.00 44.15 ATOM 5313 C GLUB 288 57.058 -4.053 63.348 1.00 44.65 ATOM 5314 O GLUB 288 55.209 -8.931 65.308 1.00 24.65 ATOM 5315 N GLYB 288 55.209 -8.931 65.308 1.00 24.55 ATOM 5316 CA GLYB 289 55.176 -6.973 66.419 1.00 24.55 ATOM 5317 C GLYB 289 55.176 -6.973 66.419 1.00 24.55 ATOM 5318 O GLYB 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLYB 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 22.2 ATOM 5320 CA VAL B 290 49.794 -5.655 68.783 1.00 120.2 ATOM 5321 CB VAL B 290 49.289 -6.504 67.629 1.00 122.2 ATOM 5322 CG1 VAL B 290 49.289 -6.504 67.629 1.00 122.2 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 122.2 ATOM 5325 O VAL B 290 51.174 -5.075 68.769 1.00 12.5 ATOM 5326 N TYR B 291 51.93 -2.941 69.346 1.00 21.5 ATOM 5327 CA TYR B 291 51.93 -2.941 69.346 1.00 21.5 ATOM 5328 CB TYR B 291 51.93 -2.941 69.346 1.00 21.0 ATOM 5329 CG TYR B 291 55.580 -2.712 66.809 1.00 19.2 ATOM 5320 CD TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5321 CB VAL B 290 49.789 -6.504 67.629 1.00 19.2 ATOM 5323 CD TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5327 CA TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5330 CD TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5330 CD TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5333 CD TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5334 CC TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5335 OH TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5337 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5337 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM 5336 C TYR B 291 55.580 -2.712 66.809 1.00 20.0 ATOM | MCYPE | 5308 | CB | GLU B | 288 | | 56.405 | -6.791 | 63.405 | 1.00 29.51 |
| ATOM 5310 CD GLU B 288 57.906 -4.769 63.347 1.00 41.1 ATOM 5311 OEI GLU B 288 57.058 -4.055 63.919 1.00 41.1 ATOM 5312 OEZ GLU B 288 59.125 -4.503 63.348 1.00 44.6 ATOM 5313 C GLU B 288 55.682 -7.819 65.527 1.00 27.8 ATOM 5314 O GLU B 288 55.682 -8.931 65.308 1.00 24.5 ATOM 5315 N GLY B 289 55.076 6-973 66.449 1.00 224.5 ATOM 5316 CA GLY B 289 55.076 6-973 66.449 1.00 224.5 ATOM 5316 CA GLY B 289 55.076 6-6.973 66.449 1.00 224.5 ATOM 5317 C GLY B 289 53.005 -5.326 66.358 1.00 26.8 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5310 CA WAL B 290 51.194 -5.079 68.440 1.00 22.3 ATOM 5321 CB VAL B 290 51.194 -5.079 68.440 1.00 22.3 ATOM 5321 CB VAL B 290 49.794 -5.655 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 49.794 -5.655 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 49.794 -5.655 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 49.794 -5.655 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 51.194 -5.079 68.440 1.00 22.3 ATOM 5326 N TYR B 291 51.722 -4.222 69.553 1.00 21.3 ATOM 5326 N TYR B 291 51.913 -7.22 -4.222 69.553 1.00 21.5 ATOM 5328 CB TYR B 291 51.913 -7.2941 69.346 1.00 21.3 ATOM 5328 CB TYR B 291 51.913 -2.941 69.346 1.00 21.3 ATOM 5329 CG TYR B 291 51.913 -2.041 69.346 1.00 21.0 ATOM 5330 CD1 TYR B 291 54.553 -2.072 68.918 1.00 21.3 ATOM 5330 CD1 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CEI TYR B 291 55.534 -2.072 68.918 1.00 21.3 ATOM 5332 CG2 VAL B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5333 CEZ TYR B 291 55.534 -2.072 68.918 1.00 21.3 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CEI TYR B 291 55.534 -2.072 68.918 1.00 21.3 ATOM 5330 CCI TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CEI TYR B 291 55.234 -3.752 67.442 1.00 23.4 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.0 20.0 20.0 20.0 20.0 20.0 20.0 | | | | | | | 57 430 | -6 003 | 62.605 | 1.00 36.06 |
| ATOM 5312 OE2 GLU B 288 57.058 -4.055 63.919 1.00 41.61 ATOM 5312 OE2 GLU B 288 59.125 -4.503 63.348 1.00 44.66 ATOM 5313 C GLU B 288 59.125 -4.503 63.348 1.00 44.66 ATOM 5314 O GLU B 288 55.209 -8.931 65.308 1.00 26.87 ATOM 5315 N GLY B 289 55.076 -6.973 66.419 1.00 24.51 ATOM 5316 CA GLY B 289 55.005 -7.326 67.204 1.00 29.1 ATOM 5316 CA GLY B 289 53.005 -5.326 66.358 1.00 24.51 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.4 ATOM 5320 CA VAL B 290 49.289 -6.504 67.629 1.00 12.2 ATOM 5321 CB VAL B 290 49.289 -6.504 67.629 1.00 12.2 ATOM 5322 CG1 VAL B 290 49.289 -6.504 67.629 1.00 12.2 ATOM 5322 CG1 VAL B 290 49.289 -6.504 67.629 1.00 12.5 ATOM 5325 CG2 VAL B 290 51.792 -4.232 69.593 1.00 21.5 ATOM 5326 N TWR B 291 51.913 -2.941 69.346 1.00 21.5 ATOM 5326 N TWR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5328 CB TWR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5328 CB TWR B 291 53.552 -1.216 69.711 1.00 21.3 ATOM 5328 CB TWR B 291 53.552 -1.216 69.711 1.00 22.6 ATOM 5331 CE1 TWR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5333 CE2 TWR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TWR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5334 CE2 TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5337 CE2 TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.2 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.0 20.0 ATOM 5336 C TWR B 291 55.500 -2.712 66.809 1.00 20.0 20.0 ATOM 5336 C TWR B 291 56.070 -3.960 68.800 1.00 20.0 20.0 ATOM 5336 C TWR B 291 56.070 -3.960 68.800 1.00 20.0 20.0 ATOM 5336 C C TWR B 292 55.604 | ATCM | | | | | | | | | |
| ATOM 5312 OE2 GUU B 288 57.058 -4.053 63.3919 1.00 41.61 ATOM 5313 C GUU B 288 55.682 -7.819 65.527 1.00 27.87 ATOM 5314 O GLU B 288 55.682 -7.819 65.527 1.00 27.87 ATOM 5315 N GLY B 289 55.176 -6.973 66.419 1.00 24.57 ATOM 5316 CA GLY B 289 55.015 -6.171 67.244 1.00 30.4 ATOM 5317 C GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -6.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.1 ATOM 5320 CA VAL B 290 48.810 -4.525 69.047 1.00 22.5 ATOM 5321 CB VAL B 290 48.810 -4.525 69.047 1.00 22.5 ATOM 5322 CG1 VAL B 290 48.810 -4.525 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 51.722 -4.232 69.593 1.00 11.5 ATOM 5325 CVAL B 290 51.724 -4.232 69.593 1.00 21.5 ATOM 5326 N TWR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5327 CA TWR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5327 CA TWR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5328 CB TWR B 291 53.552 -1.216 69.711 1.00 20.4 ATOM 5330 CD1 TWR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5330 CD1 TWR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5331 CE1 TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5333 CE2 TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5335 CH TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5335 CH TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5335 CH TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.2 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.6 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.2 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.2 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.2 ATOM 5336 CH TWR B 291 55.580 -2.712 66.899 1.00 20.2 ATOM 5336 CH TWR B 291 55.668 -0.479 70.429 1.00 20.8 ATOM 5336 CH TWR B 291 55.668 -0.479 70.429 1.00 20.2 ATOM 5346 CH DWR B 295 55.1580 -2.714 61.00 20.8 ATOM 5336 CH TWR B 291 50.668 -0.479 70.429 1.00 20. | MOTA | 5310 | CD | GLU B | 288 | | | | | |
| ## STON | | | OE1 | GLU B | 288 | | 57.058 | -4.055 | 63.919 | 1.00 41.19 |
| ATOM 5314 O GLU B 288 55.682 -7.819 65.527 1.00 27.8 ATOM 5314 O GLU B 288 55.209 -8.931 65.308 1.00 26.8 ATOM 5315 N GLY B 289 55.176 -6.973 66.419 1.00 24.5 ATOM 5316 CA GLY B 289 55.005 -7.326 67.204 1.00 29.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 26.1 ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5321 CB VAL B 290 49.794 -5.655 68.783 1.00 16.2 ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 16.2 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5324 C VAL B 290 51.722 -4.232 69.593 1.00 21.5 ATOM 5325 O VAL B 290 51.960 -4.741 70.687 1.00 21.3 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 22.1 ATOM 5327 CA TYR B 291 52.479 -2.063 70.357 1.00 21.3 ATOM 5332 CG2 TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5332 CG TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5333 CC1 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5333 CC2 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5333 CC2 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5333 CC2 TYR B 291 55.700 -1.875 67.549 1.00 20.4 ATOM 5333 CC2 TYR B 291 55.700 -1.875 67.549 1.00 20.4 ATOM 5333 CC2 TYR B 291 55.700 -1.875 67.549 1.00 20.4 ATOM 5334 CT TYR B 291 55.700 -1.875 67.549 1.00 20.2 ATOM 5335 CH TYR B 291 55.700 -1.875 67.549 1.00 20.2 ATOM 5336 C TYR B 291 55.700 -1.875 67.549 1.00 20.2 ATOM 5337 CT TYR B 291 55.700 -1.875 67.549 1.00 20.2 ATOM 5338 N LEU B 292 55.500 -2.712 66.809 1.00 20.6 ATOM 5336 C TYR B 291 56.725 -3.752 67.442 1.00 23.4 ATOM 5337 C TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5338 N LEU B 292 55.580 -2.712 67.442 1.00 23.4 ATOM 5336 C TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5337 C TYR B 291 56.235 -3.752 67.442 1.00 20.2 ATOM 5340 C B LEU B 292 49.765 -1.807 77.548 1.00 20.2 ATOM 5341 C G LEU B 292 49.765 -1.807 77.55 1.00 20.2 ATOM 5342 C D LEU B 292 55.500 -2.712 68.891 1.00 20.2 ATOM 5343 C C TYR B 291 50.00 -2.547 77.55 1.00 20.2 ATOM 5340 C B LEU B 292 55.514 68.77 77.55 1.00 20.2 A | | | | | | | | _4 503 | 63 348 | 1.00.44.69 |
| ATOM 5314 O GLU B 288 55.209 -8.931 65.308 1.00 26.5 ATOM 5315 N GLY B 289 54.006 -7.326 67.204 1.00 29.1 ATOM 5316 CA GLY B 289 54.006 -7.326 67.204 1.00 29.1 ATOM 5317 C GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5318 N VAL B 290 51.194 -5.079 68.404 1.00 22.2 ATOM 5320 CA VAL B 290 51.194 -5.079 68.404 1.00 22.2 ATOM 5320 CA VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5323 CG2 VAL B 290 49.794 -6.505 68.783 1.00 12.5 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5326 C VAL B 290 51.792 -4.232 69.593 1.00 12.5 ATOM 5326 C VAL B 290 51.792 -4.232 69.593 1.00 21.5 ATOM 5326 C VAL B 290 51.792 -4.232 69.593 1.00 21.5 ATOM 5326 N TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5327 CA TYR B 291 53.592 -1.216 69.711 1.00 20.6 ATOM 5328 CB TYR B 291 53.592 -1.216 69.711 1.00 20.6 ATOM 5330 CD1 TYR B 291 54.730 -1.875 67.549 1.00 19.5 ATOM 5333 CC2 TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5333 CC2 TYR B 291 55.524 -3.122 69.571 1.00 22.8 ATOM 5333 CC2 TYR B 291 55.234 -3.122 69.571 1.00 22.8 ATOM 5333 CC2 TYR B 291 55.234 -3.122 69.571 1.00 23.4 ATOM 5333 CC2 TYR B 291 55.235 -3.752 67.442 1.00 23.4 ATOM 5333 CC2 TYR B 291 55.235 -3.752 67.442 1.00 23.4 ATOM 5333 CC2 TYR B 291 55.235 -3.752 67.442 1.00 23.4 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 23.4 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 22.8 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 22.8 ATOM 5336 C TYR B 291 55.6070 -2.712 68.6072 1.00 22.9 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 22.8 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 22.8 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 22.9 ATOM 5336 C TYR B 291 55.255 -3.752 67.442 1.00 22.9 ATOM 5336 C TYR B 291 55.256 68.0479 79.499 1.00 20.2 ATOM 5340 C G LEU B 292 55.516 68.0479 79.499 1.00 20.2 ATOM 5340 C G LEU B 292 55.516 68.0479 79.499 1.00 20.2 ATOM 5340 C G LEU B 292 55.516 68.0479 79.916 1 | MOTA | 5312 | | | | | | | | |
| ATOM 5314 O GLU B 288 55.209 -8.931 65.308 1.00 24.5 ATOM 5315 N GLY B 289 55.176 -6.973 66.44) 1.00 24.5 ATOM 5316 CA GLY B 289 53.015 -6.171 67.244 1.00 30.4 ATOM 5317 C GLY B 289 53.015 -6.171 67.244 1.00 20.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 23.9 ATOM 5319 N VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5322 CG1 VAL B 290 48.810 -4.525 69.047 1.00 22.2 ATOM 5322 CG2 VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5323 CG2 VAL B 290 49.794 -6.504 67.629 1.00 19.2 ATOM 5324 C VAL B 290 51.960 -4.741 70.687 1.00 21.5 ATOM 5325 N TYR B 291 51.950 -4.741 70.687 1.00 21.3 ATOM 5326 C TYR B 291 53.552 -1.216 69.911 1.00 20.4 ATOM 5327 CA TYR B 291 53.552 -1.216 69.911 1.00 20.4 ATOM 5328 CB TYR B 291 53.552 -1.216 69.911 1.00 20.4 ATOM 5330 CD1 TYR B 291 55.530 -2.072 68.918 1.00 23.0 ATOM 5331 CE1 TYR B 291 55.524 -3.752 69.557 1.00 19.2 ATOM 5331 CE1 TYR B 291 55.524 -3.752 69.527 1.00 22.8 ATOM 5332 CD2 TYR B 291 55.524 -3.752 69.953 1.00 19.2 ATOM 5333 CE2 TYR B 291 55.524 -1.216 69.711 1.00 20.4 ATOM 5331 CE1 TYR B 291 55.524 -3.752 69.953 1.00 22.6 ATOM 5333 CE2 TYR B 291 55.524 -3.752 69.953 1.00 22.6 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5336 C TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5337 C GE TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5338 N LEU B 292 55.224 -3.126 69.9527 1.00 22.8 ATOM 5336 C GE TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5337 C GE TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5338 N LEU B 292 55.2540 -3.752 67.442 1.00 23.4 ATOM 5336 C GE TYR B 291 56.636 -0.479 70.429 1.00 20.2 ATOM 5336 C GE TYR B 291 56.636 -0.479 70.429 1.00 20.2 ATOM 5360 C GLY B 292 51.522 -1.204 72.399 1.00 20.7 ATOM 5360 C GLY B 292 51.522 -1.204 72.399 1.00 20.7 ATOM 5360 C GLY B 293 51.60 68.84 1.90 70.429 1.00 20.7 ATOM 5360 C GLY B 295 51.757 7.758 80.229 1.00 10.7 ATOM 5360 C GLY B 295 51.790 90.80 8 | MOTE | 5313 | С . | _GLU B | 288 | | 55.682 | -7.819 | 65.527 | |
| ATOM 5316 CA GLY B 289 55.176 -6.973 66.449 1.00 24.5 ATOM 5316 CA GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 0 GLY B 289 53.005 -6.171 67.244 1.00 30.4 ATOM 5318 0 GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.9 ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5321 CB VAL B 290 49.794 -5.655 68.738 1.00 18.2 ATOM 5322 CG1 VAL B 290 49.299 -6.504 67.629 1.00 12.6 ATOM 5323 CG2 VAL B 290 49.299 -6.504 67.629 1.00 12.5 ATOM 5323 CG2 VAL B 290 49.299 -6.504 67.629 1.00 12.5 ATOM 5326 N VAL B 290 51.194 -4.525 69.047 1.00 22.6 ATOM 5326 N VAL B 290 51.722 -4.232 69.593 1.00 21.5 ATOM 5326 N VAL B 290 51.960 -4.741 70.687 1.00 21.5 ATOM 5326 N VAL B 290 51.960 -4.741 70.687 1.00 21.5 ATOM 5326 N VAL B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5328 CB TYR B 291 53.552 -1.216 69.711 1.00 20.4 ATOM 5328 CB TYR B 291 53.552 -1.216 69.711 1.00 20.4 ATOM 5328 CB TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CEZ TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CEZ TYR B 291 55.234 -3.122 69.527 1.00 22.3 ATOM 5333 CEZ TYR B 291 55.200 -2.712 66.809 1.00 20.6 ATOM 5336 C TYR B 291 55.200 -2.712 66.809 1.00 20.6 ATOM 5338 N LEU B 292 57.007 -4.612 66.225 1.00 28.0 ATOM 5336 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5336 C TYR B 291 55.236 -3.752 67.442 1.00 23.4 ATOM 5345 C TYR B 291 55.236 -3.752 67.442 1.00 23.4 ATOM 5345 C TYR B 291 55.252 -1.204 72.399 1.00 21.7 ATOM 5340 CB LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CB LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CB LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CB LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CB LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CB LEU B 292 51.525 -1.359 77.914 1.00 22.9 ATOM 5340 CB LEU B 292 51.525 -1.00 42.6 ATOM 5345 C LEU B 292 51.525 -1.399 79.916 1.00 12.5 ATOM 5340 CB LEU B 292 51.525 -1.399 79.916 1.00 12.5 ATOM 5350 C GL | | | | CLII B | 288 | | -55 209 | -8.931 | 65.308 | 1.00 26.80 |
| ATOM 5316 CA GLY B 289 54.006 -7.326 67.200 1.00 29.1 ATOM 5317 C GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 22.2 ATOM 5320 CA VAL B 290 52.171 -6.142 68.268 1.00 22.2 ATOM 5321 CB VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 19.2 ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 19.2 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5325 O VAL B 290 51.722 -4.232 69.593 1.00 21.3 ATOM 5325 O VAL B 290 51.722 -4.232 69.593 1.00 21.3 ATOM 5325 O VAL B 290 51.722 -4.232 69.593 1.00 21.3 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.3 ATOM 5327 CA TYR B 291 51.913 -2.941 69.346 1.00 21.3 ATOM 5329 CG TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5330 CD1 TYR B 291 54.756 -2.072 68.918 1.00 23.0 ATOM 5331 CEI TYR B 291 54.756 -2.712 66.809 1.00 20.6 ATOM 5331 CEI TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CD2 TYR B 291 55.234 -3.122 69.557 1.00 22.8 ATOM 5334 CZ TYR B 291 55.234 -3.122 69.557 1.00 22.0 ATOM 5335 CD2 TYR B 291 55.234 -3.122 69.557 1.00 22.0 ATOM 5336 CD TYR B 291 55.234 -3.122 69.557 1.00 22.0 ATOM 5336 CD TYR B 291 55.234 -3.122 69.557 1.00 22.0 ATOM 5336 CD TYR B 291 55.260 -2.712 66.809 1.00 20.6 ATOM 5337 O TYR B 291 55.260 -2.712 66.809 1.00 20.6 ATOM 5334 CZ TYR B 291 55.234 -3.122 69.557 1.00 22.9 ATOM 5334 CZ TYR B 291 55.250 -2.712 66.809 1.00 20.2 ATOM 5336 CD TYR B 291 55.250 -2.712 66.809 1.00 20.2 ATOM 5336 CD TYR B 291 55.250 -2.712 66.809 1.00 20.2 ATOM 5336 CD TYR B 291 55.600 -2.712 66.809 1.00 20.2 ATOM 5336 CD TYR B 291 55.600 -2.712 66.809 1.00 20.2 ATOM 5336 CD TYR B 291 55.600 -2.712 66.809 1.00 20.2 ATOM 5336 CD TYR B 291 55.600 -2.712 66.809 1.00 20.2 ATOM 5337 O TYR B 291 55.600 -2.712 66.809 1.00 20.2 ATOM 5339 CD EUB 292 55.500 -2.712 66.809 1.00 20.2 ATOM 5339 CD EUB 292 55.500 -2.712 66.809 1.00 20.2 ATOM 5340 C EUB 292 55.500 -2.712 66.809 1.00 20.2 A | | | | | | | | | | 1 00 24 53 |
| ATOM 5316 CA GLY B 289 54.006 -7.326 67.244 1.00 29.4 ATOM 5318 O GLY B 289 53.015 -6.171 67.244 1.00 29.4 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 26.1 ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5321 CB VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG1 VAL B 290 49.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG1 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5323 CC2 VAL B 290 51.960 -4.741 70.687 1.00 22.6 ATOM 5325 O VAL B 290 51.960 -4.741 70.687 1.00 21.5 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.5 ATOM 5327 CA TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5329 CG TYR B 291 53.522 -1.216 69.711 1.00 20.4 ATOM 5320 CD TYR B 291 55.580 -2.712 66.89 10.00 23.0 ATOM 5330 CD TYR B 291 55.580 -2.712 66.89 10.00 23.0 ATOM 5331 CEI TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CEZ TYR B 291 55.000 -3.356 68.800 1.00 26.0 ATOM 5333 CEZ TYR B 291 55.000 -3.356 68.800 1.00 26.0 ATOM 5336 C TYR B 291 55.000 -3.356 68.800 1.00 26.0 ATOM 5337 C TYR B 291 55.000 -3.356 68.800 1.00 26.0 ATOM 5338 N LEUB 292 51.562 -1.264 73.375 1.00 29.3 ATOM 5338 N LEUB 292 51.665 -1.180 71.068 1.00 20.6 ATOM 5339 CA LEUB 292 51.665 -1.180 71.068 1.00 20.6 ATOM 5340 C C TYR B 291 50.668 0.479 70.429 1.00 20.5 ATOM 5341 C C LEUB 292 51.522 -1.204 72.399 1.00 22.9 ATOM 5342 C DL LEUB 292 51.522 -1.204 72.399 1.00 22.9 ATOM 5343 CD LEUB 292 51.522 -1.204 72.399 1.00 22.9 ATOM 5344 C LEUB 292 51.330 0.557 74.147 1.00 21.5 ATOM 5345 O LEUB 292 51.522 -1.204 72.299 1.00 22.9 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 22.9 ATOM 5347 CA GLY B 293 51.195 2.537 75.521 1.00 22.9 ATOM 5348 C GLY B 293 51.195 2.537 75.931 1.00 20.7 ATOM 5346 N GLY B 293 51.195 2.537 75.931 1.00 20.7 ATOM 5346 N GLY B 293 51.196 3.379 80.257 1.00 22.9 ATOM 5355 O GLY B 293 51.196 3.979 76.930 1.00 26.1 ATOM 5356 C GLY B 293 51.196 3.979 76.930 1.00 26.1 ATOM 5357 O GLY B 293 51.196 3.979 76.930 1.00 20.6 ATOM 5356 C GLY B 295 51.370 9.160 82.336 1.00 20.7 ATOM 5356 C GLY B 295 51.370 9.160 82.336 1.00 20.7 ATOM 5356 C GLY B 296 5 | MOTA | 5315 | N | GLY B | 289 | | | | | |
| ATOM 5318 O GLY B 289 53.015 -6.171 67.244 1.00 30.4 ATOM 5318 O GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 51.174 -5.079 68.268 1.00 23.9 ATOM 5321 CB VAL B 290 49.774 -5.655 68.783 1.00 12.7 ATOM 5322 CG VAL B 290 49.774 -5.655 68.783 1.00 12.7 ATOM 5323 CC2 VAL B 290 49.784 -5.655 69.047 1.00 22.2 ATOM 5323 CC2 VAL B 290 49.89 -6.504 67.629 1.00 19.2 ATOM 5323 CC2 VAL B 290 51.722 -4.232 69.593 1.00 21.3 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.3 ATOM 5326 N TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.3 ATOM 5330 CD1 TYR B 291 55.580 -2.712 66.809 1.00 21.3 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 21.3 ATOM 5332 CD2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.580 -2.712 66.809 1.00 20.2 ATOM 5334 CZ TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5335 CP2 TYR B 291 55.6070 -3.960 68.800 1.00 26.0 ATOM 5336 C TYR B 291 55.6070 -3.960 68.800 1.00 26.0 ATOM 5336 C TYR B 291 55.6064 -0.479 70.429 1.00 20.2 ATOM 5336 C TYR B 291 55.6668 -0.479 70.429 1.00 20.2 ATOM 5337 CP2 TYR B 291 55.6668 -0.479 70.429 1.00 20.2 ATOM 5339 CA LEU B 292 55.550 -0.04 -0.426 73.227 1.00 28.0 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.227 1.00 20.2 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.227 1.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.227 1.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.75 T.10 0.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.75 T.10 0.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.227 1.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.227 1.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.75 T.10 0.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.75 T.10 0.00 20.7 ATOM 5340 CB LEU B 292 55.550 -0.04 -0.426 73.75 T.10 0.00 20.7 ATOM 5350 | | 5316 | CA | GLY B | 289 | • | 54.006 | -7.326 | 67.204 | |
| ATOM 5318 0 GLY B 289 53.005 -5.326 66.358 1.00 26.1 ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.9 ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5321 CB VAL B 290 49.769 -6.504 67.629 1.00 19.2 ATOM 5322 CG1 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5326 C VAL B 290 51.722 -4.232 69.593 1.00 21.5 ATOM 5325 O VAL B 290 51.960 -4.741 70.687 1.00 21.3 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5327 CA TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5329 CG TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5330 CD1 TYR B 291 54.740 -1.875 67.549 1.00 19.2 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 23.0 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5336 C TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5337 O TYR B 291 57.027 -4.612 66.722 1.00 23.4 ATOM 5338 C C TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5338 C C TYR B 291 57.027 -4.612 66.722 1.00 23.4 ATOM 5336 C TYR B 291 57.027 -4.612 66.722 1.00 23.4 ATOM 5337 O TYR B 291 51.665 -1.180 71.068 1.00 26.8 ATOM 5338 C LEU B 292 49.765 -1.369 74.088 1.00 22.1 ATOM 5340 C LEU B 292 49.765 -1.369 74.088 1.00 22.1 ATOM 5341 C G LEU B 292 49.765 -1.369 74.088 1.00 22.3 ATOM 5342 C DL LEU B 292 51.330 0.557 74.147 1.00 21.7 ATOM 5345 O LEU B 292 51.330 0.557 74.147 1.00 21.7 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 22.3 ATOM 5347 CA GLY B 293 51.195 2.537 75.521 1.00 22.3 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 22.7 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 22.7 ATOM 5356 C GLY B 293 51.195 2.537 75.521 1.00 21.7 ATOM 5357 O GLY B 293 51.195 2.537 75.521 1.00 21.7 ATOM 5356 C GLY B 293 51.196 2.357 79.916 1.00 17.4 ATOM 5357 O GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5356 C GLY B 295 53.738 4.739 81.551 1.00 17.3 ATOM 5356 C | | | | | | | 53 015 | -6.171 | 67.244 | 1.00 30.46 |
| ATOM 5319 N VAL B 290 52.171 -6.142 68.268 1.00 23.9 ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5321 CB VAL B 290 48.810 -4.555 68.703 1.00 18.7 ATOM 5322 CG1 VAL B 290 48.810 -4.555 69.047 1.00 22.6 ATOM 5323 CG2 VAL B 290 49.289 -6.504 67.629 1.00 19.2 ATOM 5326 N TYR B 291 51.923 -2.941 69.346 1.00 21.3 ATOM 5326 N TYR B 291 51.933 -2.941 69.346 1.00 21.0 ATOM 5327 CA TYR B 291 51.933 -2.941 69.346 1.00 21.0 ATOM 5328 CB TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5328 CB TYR B 291 54.553 -2.072 68.918 1.00 20.4 ATOM 5330 CD1 TYR B 291 54.553 -2.072 68.918 1.00 20.4 ATOM 5331 CB1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5332 CD2 TYR B 291 55.234 -3.122 69.527 1.00 22.3 ATOM 5333 CD2 TYR B 291 55.234 -3.122 69.571 1.00 22.4 ATOM 5333 CD2 TYR B 291 55.234 -3.122 69.577 1.00 22.4 ATOM 5333 CD2 TYR B 291 55.234 -3.122 69.577 1.00 22.4 ATOM 5333 CD2 TYR B 291 55.234 -3.122 69.577 1.00 22.4 ATOM 5333 CD2 TYR B 291 55.234 -3.122 69.577 1.00 22.4 ATOM 5335 CD TYR B 291 55.234 -3.122 69.577 1.00 22.4 ATOM 5336 C TYR B 291 55.234 -3.122 69.577 1.00 22.4 ATOM 5337 CD TYR B 291 57.027 -4.612 66.722 1.00 23.4 ATOM 5338 N LEU B 292 50.604 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 50.604 -0.479 70.429 1.00 20.2 ATOM 5340 CB LEU B 292 50.604 -0.426 73.227 1.00 22.1 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.7 ATOM 5342 CD LEU B 292 51.330 0.557 74.147 1.00 12.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 22.9 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5347 CA GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5346 N GLY B 293 51.164 4.719 79.916 1.00 17.7 ATOM 5347 CA GLY B 293 51.263 0.755 77.113 1.00 22.9 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5347 CA GLY B 293 51.263 0.755 77.113 1.00 22.9 ATOM 5348 C GLY B 293 51.164 7.77 7.88 7.7914 1.00 24.6 ATOM 5355 N GLY B 294 51.145 4.719 79.916 1.00 17.7 ATOM 5356 C GLY B 295 51.577 4.180 82.232 1.00 10.6 ATOM 5357 O GLY B 296 51.790 9.160 82.336 1.00 20.2 ATOM 535 | ATOM | | | | | | | | | 1 00 26 17 |
| ATOM 5320 CA VAL B 290 51.194 -5.079 68.440 1.00 22.2 ATOM 5321 CB VAL B 290 48.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG1 VAL B 290 48.794 -5.655 68.783 1.00 18.7 ATOM 5322 CG2 VAL B 290 49.289 -6.504 67.629 1.00 22.6 ATOM 5325 0 VAL B 290 51.722 -4.232 69.593 1.00 21.5 ATOM 5325 0 VAL B 290 51.960 -4.741 70.687 1.00 21.5 ATOM 5326 N TYR B 291 51.933 -2.941 69.346 1.00 21.0 ATOM 5327 CA TYR B 291 51.933 -2.941 69.346 1.00 21.0 ATOM 5327 CA TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5329 CG TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5330 CD1 TYR B 291 54.740 -1.875 67.549 1.00 19.2 ATOM 5331 CE1 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CEZ TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CEZ TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5335 CF TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5336 CF TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5336 CF TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5336 CF TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5335 CF TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5335 CF TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5336 CF TYR B 291 55.260 -2.712 66.809 1.00 26.6 ATOM 5335 CF TYR B 291 55.254 -3.752 67.442 1.00 28.4 ATOM 5336 CF TYR B 291 55.6070 -3.960 68.800 1.00 26.0 ATOM 5336 CF TYR B 291 55.6064 -0.479 70.429 1.00 20.2 ATOM 5336 CF TYR B 291 55.6668 -0.479 70.429 1.00 20.2 ATOM 5340 CF LEU B 292 49.765 -1.369 74.088 1.00 20.7 ATOM 5340 CF LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CF LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CF LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CF LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5340 CF LEU B 292 51.524 73.375 1.00 22.9 ATOM 5344 CF LEU B 292 51.524 73.375 1.00 22.9 ATOM 5346 CF LEU B 292 51.524 73.375 1.00 22.9 ATOM 5346 CF LEU B 292 52.514 0.404 74.426 1.00 19.4 ATOM 5345 CF LEU B 292 51.516 30 0.557 74.411 1.00 21.0 ATOM 5346 CF LEU B 292 51.516 30 0.557 74.417 1.00 20.7 ATOM 5345 CF LEU B 292 51.516 30 0.557 74.417 1.00 20.7 ATOM 5345 CF LEU B 292 51.5177 9.758 85.90 1.00 20.7 ATOM | ATOM | 5318 | 0 | | | | | | | |
| ATOM 5321 CB VAL B 290 | 2 mOM | 5319 | N | VAL B | 290 | | 52.171 | -6.142 | 68.268 | |
| ATOM 5322 CB VAL B 290 | | | | | | | 51 194 | -5.079 | 68.440 | 1.00 22.25 |
| ATOM 5322 CG1 VAL B 290 | ATOM | | | | | | | | | |
| ATOM 5322 CG1 VAL B 290 48.810 -4.525 69.047 1.00 19.2 ATOM 5323 CG2 VAL B 290 51.722 -4.232 69.593 1.00 21.3 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5326 T CA TYR B 291 52.479 -2.063 70.357 1.00 19.5 ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5329 CG TYR B 291 54.553 -2.072 68.918 1.00 21.0 ATOM 5330 CD1 TYR B 291 54.740 -1.875 67.549 1.00 19.5 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.247 -3.960 68.800 1.00 26.8 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.8 ATOM 5335 CT TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5335 CT TYR B 291 55.686 -0.479 70.429 1.00 20.4 ATOM 5336 C TYR B 291 55.668 -0.479 70.429 1.00 20.4 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5339 CA LEU B 292 49.765 -1.369 74.088 1.00 22.0 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 22.0 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.7 ATOM 5343 CD2 LEU B 292 49.091 -2.542 73.375 1.00 22.7 ATOM 5343 CD2 LEU B 292 49.091 -2.542 73.375 1.00 22.7 ATOM 5346 N GLYB B 292 51.522 -1.204 72.289 1.00 21.7 ATOM 5346 N GLYB B 293 51.163 1.979 76.930 1.00 21.5 ATOM 5346 N GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5346 N GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5346 N GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5346 N GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 C GLYB B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5350 C GLYB B 295 51.577 4.180 82.292 1.00 10.5 ATO | ATOM | 5321 | | | | | | | | |
| ATOM 5324 C2 VAL B 290 | | 5322 | CG1 | VAL B | 290 | | 48.810 | -4.525 | 69.047 | |
| ATOM 5224 C VAL B 290 51.722 -4.232 69.593 1.00 21.5 ATOM 5325 O VAL B 290 51.960 -4.741 70.687 1.00 21.3 ATOM 5325 N TYR B 291 51.913 -2.941 69.346 1.00 21.3 ATOM 5326 N TYR B 291 52.479 -2.063 70.357 1.00 12.5 ATOM 5328 CB TYR B 291 52.479 -2.063 70.357 1.00 12.5 ATOM 5329 CG TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5330 CD1 TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.4 ATOM 5335 CH TYR B 291 55.234 -3.122 67.442 1.00 23.4 ATOM 5336 C TYR B 291 55.0604 -0.426 73.227 1.00 22.5 ATOM 5336 C TYR B 291 50.666 -0.479 70.429 1.00 20.7 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.7 ATOM 5339 CA LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5334 CC LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5334 CD LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5334 CD LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5334 CD LEU B 292 48.328 -3.362 74.411 1.00 21.7 ATOM 5336 C BLEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5344 C LEU B 292 48.342 -3.362 74.411 1.00 21.5 ATOM 5344 C LEU B 292 51.530 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5347 CA GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 20.9 ATOM 5350 N GLY B 295 51.770 1.979 91.00 20.9 ATOM 5350 N GLY B 295 51.770 1.00 | | | | | | | 49 289 | -6 504 | 67.629 | 1.00 19.26 |
| ATOM 5325 O VAL B 290 | ATOM | | | | | | | | | |
| ATOM 5325 O VAL B 290 51.960 -4.741 70.887 1.00 21.5 ATOM 5326 N TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5327 CA TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5329 CG TYR B 291 54.553 -2.072 68.918 1.00 20.4 ATOM 5330 CD1 TYR B 291 54.553 -2.072 68.918 1.00 20.4 ATOM 5331 CE1 TYR B 291 55.582 -1.216 69.711 1.00 20.4 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.5 ATOM 5332 CD2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CD2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CD2 TYR B 291 55.034 -3.122 69.527 1.00 22.8 ATOM 5333 CD2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 OH TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5336 C TYR B 291 55.6235 -3.752 67.442 1.00 23.4 ATOM 5335 OH TYR B 291 55.6235 -3.752 67.442 1.00 23.4 ATOM 5335 OH TYR B 291 55.6235 -3.752 67.442 1.00 23.4 ATOM 5337 O TYR B 291 55.6235 -3.752 67.442 1.00 23.4 ATOM 5337 O TYR B 291 55.660 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 55.580 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 55.580 -0.479 70.429 1.00 20.7 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5342 CD1 LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5343 CD2 LEU B 292 49.765 -1.369 74.147 1.00 21.5 ATOM 5345 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.5 ATOM 5345 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.5 ATOM 5345 CD2 LEU B 292 55.514 0.404 74.426 1.00 19.5 ATOM 5345 C C GLY B 293 55.606 1.571 74.613 1.00 20.5 ATOM 5346 N GLY B 293 55.606 1.571 74.613 1.00 20.5 ATOM 5345 C C GLY B 293 55.606 1.571 74.613 1.00 20.5 ATOM 5345 C C GLY B 293 55.5606 1.571 74.613 1.00 20.5 ATOM 5345 C C GLY B 293 55.163 0.765 77.133 1.00 20.5 ATOM 5355 CA GLY B 293 55.5606 1.571 74.613 1.00 20.5 ATOM 5355 CA GLY B 293 55.573 4.180 82.282 1.00 19.5 ATOM 5356 C GLY B 293 55.573 4.180 82.282 1.00 19.5 ATOM 5356 CA GLY B 295 55.574 4.199 79.916 1.00 17.3 ATOM 5356 CA GLY B 295 55.777 4.180 82.582 1.00 20.6 ATOM 5356 CA GLY B 295 55.773 8.800 82.597 79.00 20.5 ATOM 5356 CA GLY B 295 55.779 77.758 85.936 1. | ATOM | 5324 | С | | | | | | | |
| ATOM 5326 N TYR B 291 51.913 -2.941 69.346 1.00 21.0 ATOM 5328 CB TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5328 CD1 TYR B 291 54.750 -2.072 68.918 1.00 23.0 ATOM 5330 CD1 TYR B 291 54.740 -1.875 67.549 1.00 19.5 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5331 CE2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 22.3 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 22.3 ATOM 5335 CP TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CP TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5336 CP TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 CP TYR B 291 55.668 -0.479 70.429 1.00 20.2 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEUB 8292 51.522 -1.204 72.399 1.00 20.2 ATOM 5339 CA LEUB 292 55.604 -0.426 73.227 1.00 22.1 ATOM 5340 CB LEUB 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5344 C LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5345 O LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 O LEU B 292 55.514 0.404 74.266 1.00 19.9 ATOM 5345 O LEU B 292 55.514 0.404 74.426 1.00 19.9 ATOM 5345 O LEU B 292 55.514 0.404 74.261 1.00 19.9 ATOM 5345 O LEU B 292 55.514 0.404 74.426 1.00 19.9 ATOM 5345 O LEU B 292 55.514 0.404 74.266 1.00 19.9 ATOM 5345 O LEU B 292 55.514 0.404 74.266 1.00 19.9 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.514 0.404 79.281 1.00 20.7 ATOM 5345 O LEU B 292 55.51 | | 5325 | 0 | VAL B | 290 | | 51.960 | -4.741 | 70.687 | 1.00 21.32 |
| ATOM 5327 CA TYR B 291 52.479 -2.063 70.357 1.00 19.2 ATOM 5329 CG TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5329 CG TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5330 CD1 TYR B 291 55.580 -2.712 66.809 1.00 20.4 ATOM 5331 CE1 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5333 CF2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CH TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5335 CH TYR B 291 50.668 -0.479 70.429 1.00 20.6 ATOM 5336 CH TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 50.604 -0.426 73.227 1.00 22.7 ATOM 5338 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5343 CD LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5345 CD LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5345 CD LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.2 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.5 ATOM 5348 C G LEU B 292 51.330 0.755 77.133 1.00 22.9 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5348 C G LEU B 292 51.330 0.755 77.133 1.00 20.5 ATOM 5345 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5345 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5345 N GLY B 293 51.163 1.979 76.930 1.00 20.6 ATOM 5356 N GLY B 293 51.363 1.90 23.3 ATOM 5350 N GLY B 294 51.176 3.538 80.285 1.00 20.6 ATOM 5350 N GLY B 295 51.577 A LEU B 295 51.373 3.179 81.551 1.00 17.3 ATOM 5356 N GLY B 295 53.738 4.936 2.207 1.00 20.6 ATOM 5356 N GLY | | | | | | | | -2 941 | 69.346 | 1.00 21.06 |
| ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.4 ATOM 5329 CG TYR B 291 54.753 -2.072 68.918 1.00 23.0 CD TYR B 291 54.754 -1.875 67.549 1.00 23.0 CD TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 CD TYR B 291 55.580 -2.712 66.809 1.00 20.6 CD TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CZ TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5333 CZ TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CD TYR B 291 57.027 -4.612 66.722 1.00 23.0 ATOM 5335 CD TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 20.7 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 20.7 ATOM 5339 CA LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5342 CD1 LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5344 C LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 C LEU B 292 55.514 0.404 74.426 1.00 19.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5345 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5345 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5345 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5340 N GLY B 293 50.606 1.571 74.613 1.00 20.60 | MOTA | | | TIR D | 231 | | | | | |
| ATOM 5328 CB TYR B 291 53.582 -1.216 69.711 1.00 20.3 0 ATOM 5329 CG TYR B 291 54.553 -2.072 68.918 1.00 23.0 ATOM 5330 CD1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 6 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 6 ATOM 5332 CD2 TYR B 291 55.580 -3.752 67.442 1.00 23.4 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 23.4 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 23.4 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 50.668 -0.479 70.429 1.00 26.2 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 26.2 ATOM 5338 N LEUB 292 50.604 -0.426 73.227 1.00 22.7 ATOM 5339 CA LEUB 292 50.604 -0.426 73.227 1.00 22.7 ATOM 5340 CB LEUB 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEUB 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5342 CD1 LEUB 292 48.149 -2.043 72.281 1.00 22.9 ATOM 5344 C LEUB 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5345 CD LEUB 292 48.149 -2.043 72.281 1.00 21.5 ATOM 5346 N GLY B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 20.7 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 20.7 ATOM 5347 CA GLY B 293 51.163 1.979 76.930 1.00 26.7 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 26.7 ATOM 5349 O GLY B 293 51.163 1.979 77.914 1.00 21.5 ATOM 5350 N GLY B 293 51.163 1.979 77.913 1.00 20.7 ATOM 5350 N GLY B 293 51.163 1.979 79.916 1.00 17.4 ATOM 5351 CA GLY B 293 51.163 1.979 79.916 1.00 17.4 ATOM 5355 CA GLY B 293 51.163 1.979 79.916 1.00 20.7 ATOM 5350 N GLY B 293 51.163 1.979 79.916 1.00 20.6 ATOM 5350 N GLY B 293 51.163 1.979 79.916 1.00 20.6 ATOM 5350 N GLY B 293 51.163 1.979 79.916 1.00 20.6 ATOM 5350 N GLY B 293 51.163 1.979 91.00 20.7 ATOM 5350 N GLY B 294 50.910 91.00 20.8 ATOM 5350 N GLY B 295 53.738 8.748 82.232 1.00 19.5 ATOM 5350 C GLY B 295 53.738 8.750 82.257 1.00 20.6 ATOM 5350 C GLY B 295 53.738 8.750 82.257 1.00 20.6 ATOM 5350 C GLY B 295 53.738 8.750 82.257 1.00 | MOTA | 5327 | CA | TYR B | 291 | | 52.4/9 | | | 1.00 19.29 |
| ATOM 5329 CG TYR B 291 54.553 -2.072 68.918 1.00 23.0 (A) ATOM 5330 CD1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 (A) ATOM 5331 CC2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 (A) ATOM 5333 CC2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 (A) ATOM 5333 CC2 TYR B 291 56.235 -3.752 67.442 1.00 23.4 (A) ATOM 5335 OH TYR B 291 56.235 -3.752 67.442 1.00 23.4 (A) ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 (A) ATOM 5336 C TYR B 291 50.668 -0.479 70.429 1.00 20.2 (A) ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 (A) ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 20.2 (A) ATOM 5339 CA LEU B 292 51.522 -1.204 72.399 1.00 20.2 (A) ATOM 5340 CB LEU B 292 49.091 -2.542 73.375 1.00 22.9 (A) ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 (A) ATOM 5343 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.0 (A) ATOM 5343 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.0 (A) ATOM 5343 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.0 (A) ATOM 5346 CD2 LEU B 292 52.514 0.404 74.426 1.00 19.5 (A) ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 (A) ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 (A) ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5349 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 293 50.606 1.571 74.613 1.00 20.9 (A) ATOM 5350 N GLY B 295 50.573 80.2 (A) ATOM 5350 N GLY B 295 50.577 4.180 82.582 1.00 16.5 (A) ATOM 5350 N GLY B 295 50.577 4.180 82.582 1.00 19.5 (A) ATOM 5350 N GLY B 295 50.577 4.180 82.582 1.00 19.5 (A) ATOM 5350 | | 5328 | CB | TYR B | 291 | | 53.582 | -1.216 | 69.711 | 1.00 20.40 |
| ATOM 5330 CD1 TYR B 291 54.740 -1.875 67.549 1.00 19.5 ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5332 CD2 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5333 CE2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5337 O TYR B 291 51.465 -1.180 71.068 1.00 26.8 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5338 N LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5340 CB LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5340 CD LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5344 C LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5345 CD2 LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 20.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 20.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 20.2 ATOM 5350 N GLY B 295 50.573 88.508 80.285 1.00 20.2 ATOM 5350 C GLY B 296 50.407 79.293 1.00 20.2 ATOM 5350 C GLY B 296 50.407 79.293 1.00 | | | | | | | 54 553 | -2 072 | 68.918 | 1.00 23.09 |
| ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.6 ATOM 5332 CD2 TYR B 291 55.234 -3.122 69.527 1.00 22.8 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CZ TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CZ TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5335 OH TYR B 291 57.027 -4.612 66.702 1.00 26.0 ATOM 5337 O TYR B 291 57.027 -4.612 66.722 1.00 26.0 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 22.7 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 22.7 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 O LEU B 292 51.330 0.557 74.147 1.00 21.0 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5348 C GLY B 293 50.606 1.571 74.613 1.00 26.1 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 26.7 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 26.7 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 CA GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5356 C GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5360 C GLY B 295 53.738 4.737 81.732 1.00 20.7 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.7 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.7 ATOM 5360 C GLY B 296 53.573 8.759 82.579 1.00 20.7 ATOM 5360 C GLY B 296 53.573 8.759 82.579 1.00 20.7 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 19.5 ATOM 5366 CD TYR B 297 53.055 88.509 1.00 21.5 ATOM 5366 CD TYR B 297 53.055 88.509 1.00 | MOTA | 5329 | | | | | | | | |
| ATOM 5331 CE1 TYR B 291 55.580 -2.712 66.809 1.00 20.8 ATOM 5332 CD2 TYR B 291 55.580 -2.712 66.800 1.00 26.0 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 CP TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5335 CP TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 51.465 -1.180 71.068 1.00 26.8 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 21.7 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5339 CA LEU B 292 49.064 -0.426 73.227 1.00 22.1 ATOM 5340 CB LEU B 292 49.065 -1.369 74.088 1.00 20.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5344 C LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 O LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5345 N GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5345 N GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5345 N GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5354 N GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 N GLY B 294 51.176 3.538 80.285 1.00 20.7 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.7 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 10.5 ATOM 5356 C GLY B 295 51.373 3.179 81.551 1.00 17.2 ATOM 5356 C GLY B 295 51.373 3.179 81.551 1.00 17.2 ATOM 5356 C GLY B 295 51.373 3.179 81.551 1.00 17.2 ATOM 5356 C GLY B 295 51.373 8.752 9.402 83.682 1.00 16.5 ATOM 5356 C GLY B 295 52.6695 5.145 82.232 1.00 16.5 ATOM 5356 C GLY B 296 52.869 8.750 82.759 1.00 20.5 ATOM 5366 C GLY B 296 52.869 8.750 82.759 1.00 20.5 ATOM 5366 C GLY B 296 52.869 8.750 82.759 1.00 20.5 ATOM 5366 CD TYR B 297 53.055 8.859 1.00 21.9 ATOM 5366 CD TYR B 297 53.055 8.859 1.00 21.9 ATOM 5366 CD TYR B 297 53.653 8.850 85.849 1. | ATOM | 5330 | CD1 | TYR B | 291 | | | | | |
| ATOM 5332 CD2 TYR B 291 55.234 -3.122 69.527 1.00 22.0 ATOM 5333 CE2 TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5334 CZ TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 51.465 -1.180 71.068 1.00 26.8 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 50.604 -0.426 73.227 1.00 22.7 ATOM 5339 CA LEU B 292 50.604 -0.426 73.227 1.00 22.7 ATOM 5340 CB LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5341 CG LEU B 292 48.328 -3.362 74.411 1.00 20.9 ATOM 5344 C LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5344 C LEU B 292 48.149 -2.043 72.281 1.00 21.5 ATOM 5345 O LEU B 292 51.530 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5340 O GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5345 O GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5345 O GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5345 O GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5345 O GLY B 293 51.163 1.979 76.930 1.00 26.9 ATOM 5350 N GLY B 294 50.980 2.407 79.293 1.00 20.7 ATOM 5350 N GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 C GLY B 295 51.577 4.180 82.582 1.00 16.3 ATOM 5355 C GLY B 295 51.577 4.180 82.582 1.00 16.3 ATOM 5355 C GLY B 295 53.738 4.737 81.732 1.00 16.3 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 21.5 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 21.5 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 22.5 ATOM 5360 C GLY B 295 53.738 4.737 81.732 1.00 16.3 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 22.5 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 22.5 ATOM 5366 CD TYR B 297 53.025 10.598 84.306 1.00 20.5 ATOM 5366 CD TYR B 297 53.025 10.598 84.306 1.00 20.5 ATOM 5366 CD TYR B 297 53.025 10.598 84.306 | | 5331 | CEI | TYR B | 291 | | 55.580 | -2.712 | 66.809 | |
| ATOM 5333 CEZ TYR B 291 56.070 -3.960 68.800 1.00 26.0 ATOM 5334 CZ TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 51.465 -1.180 71.068 1.00 26.8 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 22.7 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 22.7 ATOM 5339 CA LEU B 292 49.765 -1.369 74.088 1.00 22.9 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 22.9 ATOM 5341 CG LEU B 292 49.765 -1.369 74.088 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5345 O LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 O LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 22.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 22.5 ATOM 5347 CA GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5345 C GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5351 CA GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5351 CA GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5352 C GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.3 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.3 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.3 ATOM 5356 C GLY B 295 51.373 3.179 81.551 1.00 17.3 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 16.3 ATOM 5356 C GLY B 295 53.738 4.737 81.732 1.00 20.5 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 16.3 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 19.5 ATOM 5366 CD TYR B 297 53.653 8.850 85.849 1.00 20.5 ATOM 5366 CD TYR B 297 53.653 8.850 85.849 1.00 20.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.996 1.00 21.9 ATOM 5366 CD TYR B 297 52.779 7.758 85.991 1.00 19.5 ATOM 5366 CD TYR B 297 52.779 | | | | | | | | | 69.527 | 1.00 22.98 |
| ATOM 5333 CZ TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5339 CA LEU B 292 50.604 -0.426 73.227 1.00 22.1 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5344 C LEU B 292 48.499 -2.043 72.281 1.00 18.0 ATOM 5344 C LEU B 292 48.49 -2.043 72.281 1.00 18.0 ATOM 5345 O LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5348 C GLY B 293 51.195 2.537 75.521 1.00 20.7 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 21.5 ATOM 5351 CA GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 20.6 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 20.6 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 52.695 51.455 82.232 1.00 19.5 ATOM 5355 CA GLY B 295 52.695 51.455 82.232 1.00 19.5 ATOM 5355 CA GLY B 295 52.695 51.456 82.207 1.00 20.6 ATOM 5355 CA GLY B 295 52.695 51.456 82.207 1.00 20.6 ATOM 5356 C GLY B 295 52.695 51.456 82.207 1.00 20.6 ATOM 5366 CD TYR B 297 53.733 4.4737 81.732 1.00 16.5 ATOM 5366 CD TYR B 297 53.073 9.402 83.682 1.00 20.4 ATOM 5366 CD TYR B 297 52.731 10.284 85.974 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.974 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.906 1.00 21.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.885 85.821 1.00 19.5 ATOM 5366 CD TYR B 297 | ATOM | | | | | | | | | |
| ATOM 5334 CZ TYR B 291 56.235 -3.752 67.442 1.00 23.4 ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 21.7 ATOM 5338 N LEU B 292 50.604 -0.426 73.227 1.00 21.7 ATOM 5339 CA LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5343 CD2 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5344 C LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5345 O LEU B 292 52.514 0.404 74.426 1.00 19.5 ATOM 5345 O LEU B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5347 CA GLY B 293 50.606 1.571 74.613 1.00 20.7 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 20.7 ATOM 5350 N GLY B 293 51.263 0.765 77.133 1.00 20.7 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 C GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 C GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 C GLY B 295 52.695 51.458 82.232 1.00 19.5 ATOM 5356 C GLY B 295 52.695 51.458 82.232 1.00 19.5 ATOM 5360 C GLY B 295 52.695 51.458 82.232 1.00 19.5 ATOM 5361 O GLY B 296 53.448 7.465 82.207 1.00 20.4 ATOM 5365 C GLY B 295 52.695 51.458 82.232 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.974 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.974 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.974 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 19.5 ATOM 5366 CD TYR B 297 52.648 85.885 85.885 1.00 20.5 ATOM 5366 CD TYR B 297 52.731 10.2 | ATOM | 5333 | CEZ | TYR B | 291 | | | | | |
| ATOM 5335 OH TYR B 291 57.027 -4.612 66.722 1.00 28.0 ATOM 5336 C TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5339 CA LEU B 292 50.604 -0.426 73.227 1.00 22.1 ATOM 5340 CB LEU B 292 49.065 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.349 -2.043 72.281 1.00 18.0 ATOM 5345 O LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.9 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.9 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5355 CA GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5350 N GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5350 N GLY B 295 53.738 4.737 81.732 1.00 16.5 ATOM 5355 CA GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5356 C GLY B 295 53.738 4.737 81.732 1.00 20.6 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5366 CD TYR B 297 53.025 10.598 84.306 1.00 23.3 ATOM 5366 CD TYR B 297 52.779 7.758 85.936 1.00 20.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.936 1.00 20.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.936 1.00 20.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.930 1.00 20.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.931 1.00 19.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.931 1.00 19.5 ATOM 5366 CD TYR B 297 52.779 7.7 | | | C7. | TYR B | 291 | | 56.235 | -3.752 | 67.442 | 1.00 23.44 |
| ATOM 5335 C TYR B 291 51.465 -1.180 71.068 1.00 26.8 ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 50.6604 -0.426 73.227 1.00 22.1 ATOM 5339 CA LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5343 CD2 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5344 C LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5345 O LEU B 292 52.514 0.404 74.426 1.00 19.9 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5348 C GLY B 293 51.195 2.537 75.521 1.00 20.7 ATOM 5349 O GLY B 293 51.263 0.765 77.133 1.00 20.9 ATOM 5349 O GLY B 293 51.263 0.765 77.133 1.00 20.9 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 N GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 N GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 N GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 C GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 C GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5356 N GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5356 N GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.4 ATOM 5361 O GLY B 296 53.448 7.465 82.207 1.00 20.4 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.4 ATOM 5366 CD TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.902 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 8 | | | | | | | | -4 612 | 66.722 | 1.00 28.02 |
| ATOM 5337 O TYR B 291 50.668 -0.479 70.429 1.00 20.2 ATOM 5338 N LEU B 292 50.604 -0.426 72.399 1.00 21.5 ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 22.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 CD2 LEU B 292 50.606 1.571 74.613 1.00 21.5 ATOM 5345 O LEU B 292 50.606 1.571 74.613 1.00 23.3 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.3 ATOM 5347 CA GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5349 O GLY B 293 51.263 0.765 77.133 1.00 20.7 ATOM 5349 O GLY B 293 51.263 0.765 77.133 1.00 20.6 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 20.6 ATOM 5351 CA GLY B 294 51.017 2.859 77.914 1.00 20.6 ATOM 5352 C GLY B 294 51.176 3.538 80.285 1.00 20.6 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.6 ATOM 5355 CA GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5357 O GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5358 N GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 16.5 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 20.6 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 20.6 ATOM 5361 O GLY B 296 52.467 6.430 82.497 1.00 20.6 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 20.6 ATOM 5366 CD TYR B 297 52.731 10.284 85.704 1.00 19.5 ATOM 5366 CD TYR B 297 52.041 8.944 85.900 1.00 24.6 ATOM 5366 CD TYR B 297 52.779 7.758 85.936 1.00 20.6 ATOM 5366 CD TYR B 297 52.779 7.758 85.936 1.00 20.6 ATOM 5366 CD TYR B 297 52.779 7.75 | ATOM | 2332 | | | | | | | | |
| ATOM 5337 O TYR B 291 | MOTA | 5336 | C | TYR B | 291 | | 51.465 | | | |
| ATOM 5338 N LEU B 292 51.522 -1.204 72.399 1.00 21.7 ATOM 5339 CA LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.0 ATOM 5343 CD2 LEU B 292 48.149 -2.043 72.281 1.00 18.0 ATOM 5345 C LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5346 N GLY B 293 51.395 0.597 74.147 1.00 21.5 ATOM 5346 N GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5349 C GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5349 O GLY B 293 51.263 0.765 77.133 1.00 20.9 ATOM 5350 N GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5351 CA GLY B 294 51.017 2.859 77.914 1.00 24.6 ATOM 5353 O GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5353 N GLY B 294 51.176 3.538 80.285 1.00 20.5 ATOM 5355 CA GLY B 294 51.145 4.719 79.916 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5356 C GLY B 296 52.695 5.145 82.232 1.00 19.5 ATOM 5360 C GLY B 296 52.869 8.750 82.759 1.00 20.6 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.6 ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.4 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5366 CB TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5366 CB TYR B 297 52.741 8.944 85.900 1.00 24.6 ATOM 5366 CD1 TYR B 297 52.741 8.944 85.900 1.00 24.6 ATOM 5366 CD1 TYR B 297 52.741 8.944 85.901 1.00 24.6 ATOM 5366 CD1 TYR B 297 52.741 8.944 85.901 1.00 24.6 ATOM 5366 CD1 TYR B 297 52.741 8.944 85.901 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.741 8.944 85.901 1.00 19.5 ATOM 5366 CD2 TYR B 297 52.741 8.944 85.902 1.00 19.5 ATOM 5366 CD2 TYR B 297 52.741 8.944 85.902 1.00 19.5 ATOM 5366 CD2 TYR B 297 52.741 8.944 85.902 1.00 19.5 ATOM 5366 CD2 TYR B 297 52.741 8.944 85.902 1.00 19.5 ATOM 5368 CD2 TYR B 297 52.741 8.944 85.902 1.00 19.5 ATOM 5368 CD2 TYR B 297 52.74 | | | Ω | TYR B | 291 | | 50.668 | -0.479 | 70.429 | 1.00 20.26 |
| ATOM 5338 N LEU B 292 | | | | | | | | -1 204 | 72.399 | 1.00 21.75 |
| ATOM 5340 CB LEU B 292 49.765 -1.369 74.088 1.00 20.9 ATOM 5341 CG LEU B 292 49.091 -2.542 73.375 1.00 22.9 ATOM 5342 CD1 LEU B 292 48.328 -3.362 74.411 1.00 21.5 ATOM 5343 CD2 LEU B 292 48.328 -3.362 74.411 1.00 21.5 ATOM 5344 C LEU B 292 48.328 -3.362 74.411 1.00 21.5 ATOM 5344 C LEU B 292 51.330 0.557 74.147 1.00 21.5 ATOM 5345 O LEU B 292 52.514 0.404 74.426 1.00 19.9 ATOM 5346 N GLY B 293 50.606 1.571 74.613 1.00 23.7 ATOM 5346 N GLY B 293 51.195 2.537 75.521 1.00 20.7 ATOM 5348 C GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5349 O GLY B 293 51.163 1.979 76.930 1.00 26.1 ATOM 5350 N GLY B 293 51.263 0.765 77.133 1.00 20.9 ATOM 5350 N GLY B 294 50.980 2.407 79.914 1.00 24.6 ATOM 5351 CA GLY B 294 50.980 2.407 79.293 1.00 20.0 ATOM 5355 C GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 N GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 16.5 ATOM 5357 O GLY B 296 52.467 6.430 82.497 1.00 20.6 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 20.6 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 20.6 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.6 ATOM 5361 O GLY B 296 52.869 8.750 82.759 1.00 20.6 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.6 ATOM 5366 CD TYR B 297 53.573 9.402 83.682 1.00 20.4 ATOM 5367 CEI TYR B 297 52.779 7.758 85.996 1.00 21.5 ATOM 5366 CD TYR B 297 52.779 7.758 85.996 1.00 20.8 ATOM 5367 CEI TYR B 297 52.779 7.758 85.996 1.00 20.8 ATOM 5368 CD2 TYR B 297 52.779 7.758 85.996 1.00 20.8 ATOM 5368 CD2 TYR B 297 52.653 8.850 85.849 1.00 20.8 ATOM 5368 CD2 TYR B 297 52.6653 8.850 85.849 1.00 20.8 ATOM 5368 CD2 TYR B 297 50.6653 8.850 85.849 1.00 20.8 ATOM 5368 CD2 TYR B 297 50.6653 8.850 85.849 1.00 20.8 ATOM 5368 CD2 TYR B 297 50.6653 8.850 85.849 1.00 20.8 | ATOM | | | | | | | | | |
| ATOM 5340 CB LEU B 292 | ATOM | 5339 | CA | | | | | | | |
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| ATOM 5352 C GLY B 294 51.176 3.538 80.285 1.00 22.5 ATOM 5353 O GLY B 294 51.145 4.719 79.916 1.00 17.4 ATOM 5354 N GLY B 295 51.373 3.179 81.551 1.00 17.4 ATOM 5355 CA GLY B 295 52.695 5.145 82.232 1.00 16.5 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5357 O GLY B 295 53.738 4.737 81.732 1.00 16.3 ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.5 ATOM 5359 CA GLY B 296 52.467 6.430 82.497 1.00 21.5 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.0 ATOM 5361 O GLY B 296 52.869 8.750 82.759 1.00 22.4 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5364 CB TYR B 297 53.025 10.598 84.306 1.00 23.4 ATOM 5366 CD TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD TYR B 297 52.731 10.284 85.936 1.00 21.5 ATOM 5366 CD TYR B 297 52.748 6.514 85.912 1.00 19.5 ATOM 5367 CEI TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TY | | | | OUI D | 204 | | | | | 1.00 20.00 |
| ATOM 5352 C GLY B 294 51.176 3.538 80.285 1.00 22.4 ATOM 5353 O GLY B 294 51.145 4.719 79.916 1.00 17.4 ATOM 5354 N GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5357 O GLY B 295 53.738 4.737 81.732 1.00 16.3 ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5359 CA GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5360 C GLY B 296 52.467 6.430 82.497 1.00 20.4 ATOM 5361 O GLY B 296 52.869 8.750 82.759 1.00 20.4 ATOM 5362 N TYR B 296 51.790 9.160 82.336 1.00 20.4 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 20.4 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5366 CD2 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.6 | ATOM | 5351 | ÇA | GLY B | 234 | | | | | |
| ATOM 5353 O GLY B 294 51.145 4.719 79.916 1.00 17.4 ATOM 5354 N GLY B 295 51.373 3.179 81.551 1.00 17.1 ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.3 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5357 O GLY B 295 53.738 4.737 81.732 1.00 19.5 ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5359 CA GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5360 C GLY B 296 53.448 7.465 82.207 1.00 20.0 ATOM 5361 O GLY B 296 52.869 8.750 82.759 1.00 22.4 ATOM 5362 N TYR B 296 51.790 9.160 82.336 1.00 20.0 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.9 ATOM 5364 CB TYR B 297 53.025 10.598 84.306 1.00 23.4 ATOM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.9 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 | | 5352 | С | GLY B | 294 | | | 3.538 | | 1.00 42.33 |
| ATCM 5354 N GLY B 295 51.373 3.179 81.551 1.00 17.1 ATCM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATCM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATCM 5357 O GLY B 295 53.738 4.737 81.732 1.00 16.3 ATCM 5358 N GLY B 296 52.467 6.430 82.497 1.00 20.0 ATCM 5359 CA GLY B 296 53.448 7.465 82.207 1.00 20.0 ATCM 5360 C GLY B 296 52.869 8.750 82.759 1.00 20.0 ATCM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.0 ATCM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.0 ATCM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.0 ATCM 5364 CB TYR B 297 53.025 10.598 84.306 1.00 23.2 ATCM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.0 ATCM 5366 CD1 TYR B 297 52.731 10.284 85.774 1.00 19.0 ATCM 5366 CD1 TYR B 297 52.731 8.944 85.900 1.00 24.0 ATCM 5366 CD2 TYR B 297 52.779 7.758 85.936 1.00 21.0 ATCM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.0 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.0 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 20.0 ATCM 5368 CD2 TY | | | | CLV B | 294 | | 51.145 | 4.719 | 79.916 | 1.00 17.46 |
| ATCM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 16.5 ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.5 ATOM 5357 O GLY B 295 53.738 4.737 81.732 1.00 16.3 ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5359 CA GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5360 C GLY B 296 52.869 8.750 82.759 1.00 20.0 ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.4 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.4 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 20.4 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.731 8.944 85.900 1.00 24.5 ATOM 5367 CE1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 20.5 ATOM 5368 CD2 TYR B | | | | GDI D | 205 | | | | | |
| ATOM 5355 CA GLY B 295 51.577 4.180 82.582 1.00 10.581 10.582 1.00 | ATOM | 5354 | N | GLY B | 233 | | | | | |
| ATOM 5356 C GLY B 295 52.695 5.145 82.232 1.00 19.53 ATOM 5357 O GLY B 295 53.738 4.737 81.732 1.00 16.33 ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.53 ATOM 5359 CA GLY B 296 53.448 7.465 82.207 1.00 20.63 ATOM 5360 C GLY B 296 52.869 8.750 82.759 1.00 22.23 ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.63 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.63 ATOM 5363 CA TYR B 297 53.573 9.402 83.682 1.00 20.63 ATOM 5364 CB TYR B 297 53.025 10.598 84.306 1.00 23.23 ATOM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.63 ATOM 5366 CD1 TYR B 297 52.731 10.284 85.900 1.00 24.63 ATOM 5366 CD1 TYR B 297 52.748 6.514 85.912 1.00 19.63 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.63 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.63 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.63 | | 5355 | CA | GLY B | 295 | | 51.577 | 4.180 | | 1.00 10.32 |
| ATOM 5357 O GLY B 295 53.738 4.737 81.732 1.00 16.3 ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.9 ATOM 5359 CA GLY B 296 53.448 7.465 82.207 1.00 20.0 ATOM 5360 C GLY B 296 52.869 8.750 82.759 1.00 22.2 ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.4 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.4 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 20.5 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5366 CD1 TYR B 297 52.731 8.944 85.900 1.00 24.5 ATOM 5366 CD1 TYR B 297 52.748 6.514 85.912 1.00 19.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8550 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8550 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8550 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8550 85.849 1.00 20.5 ATOM 5368 | | | | CLV P | 295 | | 52.695 | 5.145 | 82.232 | |
| ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.5 ATOM 5359 CA GLY B 296 53.448 7.465 82.207 1.00 20.0 ATOM 5360 C GLY B 296 52.869 8.750 82.759 1.00 22.2 ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.0 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.2 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.2 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 | | | | GDI D | 205 | | | | | 1.00 16.31 |
| ATOM 5358 N GLY B 296 52.467 6.430 82.497 1.00 21.00 10.00 1 | ATOM | 5357 | 0 | | | | | | | |
| ATCM 5359 CA GLY B 296 53.448 7.465 82.207 1.00 20.00 ATCM 5360 C GLY B 296 52.869 8.750 82.759 1.00 22.00 ATCM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.00 ATCM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.00 ATCM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.00 ATCM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.00 ATCM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.00 ATCM 5366 CD1 TYR B 297 52.79 7.758 85.936 1.00 21.00 ATCM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.00 ATCM 5368 CD2 TYR B | | 5358 | N | | | | 52.467 | | 84.49/ | |
| ATCM 5360 C GLY B 296 52.869 8.750 82.759 1.00 22.2 ATCM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.4 ATCM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.5 ATCM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.2 ATCM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATCM 5365 CG TYR B 297 52.731 10.284 85.774 1.00 19.5 ATCM 5366 CD1 TYR B 297 52.79 7.758 85.936 1.00 24.5 ATCM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATCM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 A | | | | | | | 53.448 | 7.465 | 82.207 | 1.00 20.05 |
| ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.4 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.2 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.5 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 | | | | 201 0 | 206 | | | | | 1.00 22.20 |
| ATOM 5361 O GLY B 296 51.790 9.160 82.336 1.00 20.5 ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.5 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.4 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.4 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.840 TY | ATOM | 5360 | C | | | | | | | 1 00 20 49 |
| ATOM 5362 N TYR B 297 53.573 9.402 83.682 1.00 20.3 ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.3 ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.3 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.3 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.3 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.3 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.3 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.3 | | 5361 | 0 | GLY B | 296 | | 51.790 | | | 1.00 20.40 |
| ATOM 5363 CA TYR B 297 53.025 10.598 84.306 1.00 23.2 ATOM 5363 CA TYR B 297 52.731 10.284 85.774 1.00 19.5 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.5 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 53 | | | | ם פעיד | 297 | | 53.573 | 9.402 | 83.682 | 1.00 20.93 |
| ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1.00 19.50 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.50 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.50 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.50 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.50 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.50 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.50 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.50 ATOM 5368 CD2 TYR B 297 50.653 85.840 1.00 19.50 ATOM 5368 CD2 TYR B 297 50.653 85.840 ATOM 5368 CD2 TYR B 297 50.653 85.840 ATOM 5368 CD2 TYR B 297 50.653 85.840 ATOM 5368 CD2 TYR B 297 50.840 | | | | 114 0 | 207 | | | | | 1.00 23.25 |
| ATOM 5364 CB TYR B 297 52.731 10.284 85.774 1100 124.7 ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.7 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.9 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.7 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.6 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.7 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.7 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.7 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.7 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.7 ATOM 5568 CD2 TYR B 297 50.653 85.849 1.00 19.7 AT | ATOM | 5363 | CA | TYR B | 271 | | | | | 1 00 10 93 |
| ATOM 5365 CG TYR B 297 52.041 8.944 85.900 1.00 24.5 ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5367 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.6 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 85.840 | | 5364 | CB | TYR 3 | 297 | | 52.731 | | | 1.00 13.77 |
| ATOM 5366 CD1 TYR B 297 52.779 7.758 85.936 1.00 21.5 ATOM 5366 CD1 TYR B 297 52.148 6.514 85.912 1.00 19.5 ATOM 5367 CE1 TYR B 297 50.653 8.850 85.849 1.00 20.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 | | | | TYP P | 297 | | 52.041 | 8.944 | 85.900 | 1.00 24.76 |
| ATOM 5366 CE1 TYR B 297 52.148 6.514 85.912 1.00 19.7 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.8 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATOM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 19.5 ATOM | | | | 111 2 | 207 | | | | | 1.00 21.97 |
| ATCM 5367 CE1 TYR B 297 52.148 6.514 65.912 1.00 120.6 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20.6 ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 120.6 | ATOM | 5366 | CDI | TYR B | 271 | | | | | 1 00 10 79 |
| ATCM 5368 CD2 TYR B 297 50.653 8.850 85.849 1.00 20. | | 5367 | CE1 | TYR B | 297 | | 52.148 | | | 1.00 10.75 |
| ATCH 3300 GP2 TWD D 207 50 012 7 612 85.822 1.00 19.5 | | | CD2 | TYR B | 297 | | 50.653 | 8.850 | 85.849 | 1.00 20.86 |
| ATOM 5369 CE2 TYR B 297 50.012 7.012 55102 1100 55 | | | CD2 | 110 0 | 207 | | | | | 1.00 19.57 |
| • | ATOM | 5369 | CE2 | TYR B | 291 | | 20.012 | 1.012 | | |
| | | | | | | | | | • | |

| | ATO: | M 5370 | CZ TYR B 2 | 97 | 50.7 | 50 | CD 05 0 | |
|---|--------|---------|---------------|----|--------|---------|----------|---------------|
| | ATO: | M 5371 | OH TYR B 2 | | 50.1 | · · · | | |
| | ATO | | | | 50.1 | ` | : | |
| | ATO | | O TYR B 2 | | 53.8 | | | 31 1.00 25.22 |
| | ATO | | N HIS B 2 | | 53.45 | | | 05 1.00 21.77 |
| | ATO | | | | 54.97 | 74 11.7 | 94 83.49 | 7 1.00 23.21 |
| | ATO | | | | 55.78 | | 76 83.27 | |
| | | | CB HIS B 2 | 98 | 57.27 | 70 12.7 | | 4 1.00 22.88 |
| | ATO | - | CG HIS B 29 | 98 | 58.09 | 7 13.9 | | 2 1.00 25.13 |
| | ATO | | CD2 HIS B 29 | 98 | 58.40 | 6 14.79 | | |
| | ATON | | ND1 HIS B 29 | 8 | 58.61 | | | |
| | MOTA | | CE1 HIS B 29 | 8 | 59.20 | | | |
| | ATOM | 1 5381 | NE2 HIS B 29 | 8 | 59.09 | | | |
| | ATOM | 5382 | C HIS B 29 | | 55.58 | | | |
| | ATOM | 5383 | O HIS B 29 | R | 56.08 | | 7 81.79 | |
| | ATOM | 5384 | N PRO B 29 | 0 | | | | |
| | ATOM | | CD PRO B 29 | 0 | 54.90 | | | |
| | ATOM | | CA PRO B 29 | | 54.38 | | | 7 1.00 29.91 |
| | ATOM | | | | 54.61 | | | 7 1.00 26.53 |
| | ATOM | - | | | 53.95 | | 2 80.343 | 2 1.00 27.76 |
| | ATOM | | CG PRO B 29 | 9 | 54.58 | | 6 81.65 | 5 1.00 27.97 |
| | | | C PRO B 29 | | 55.81 | | 0 79.19 | 1.00 27.08 |
| | ATOM | | O PRO B 29 | 9 | 55.73 | B 14.47 | 2 78.05 | |
| | ATOM | | N TYR B 30 | 0 | 56.92 | 5 15.48 | 4 79.668 | 1.00 27.30 |
| | ATOM | 5392 | CA TYR B 30 | | 58.114 | | | |
| | MOTA | 5393 | CB TYR B 300 | 0 | 59.173 | | 6 79.466 | |
| | MOTA | 5394 | CG TYR B 300 |) | 58.684 | | | |
| | MOTA | 5395 | CD1 TYR B 300 |) | 57.414 | | 79.921 | |
| | MOTA | 5396 | CE1 TYR B 300 | | 56.971 | 19.568 | | |
| | ATOM | 5397 | CD2 TYR B 300 | | 59.499 | | | |
| | ATOM | 5398 | CE2 TYR B 300 | | 59.072 | | | |
| | ATOM | 5399 | CZ TYR B 300 | | | | | |
| | MOTA | | OH TYR B 300 | | 57.808 | | | |
| | ATOM | | C TYR B 300 | | 57.374 | | | 1.00 43,90 |
| | ATOM | | O TYR B 300 | | 58.731 | | | 1.00 25.20 |
| | ATOM | | N ALA B 300 | | 59.106 | | 77.445 | 1.00 25.15 |
| | ATOM | | | | 58.845 | | 79.628 | 1.00 20.55 |
| | ATOM | | | | 59.414 | 12.080 | 79.508 | 1.00 22.12 |
| | ATOM | | | | 59.417 | 11.388 | 80.874 | 1.00 17.09 |
| | ATOM | | C ALA B 301 | | 58.608 | 11.260 | 78.505 | 1.00 15.20 |
| | | | ALA B 301 | | 59.161 | 10.629 | 77.613 | 1.00 17.12 |
| | ATOM | _ | LEU B 302 | | 57.295 | 11.290 | 78.667 | 1.00 18.02 |
| | ATOM | | CA LEU B 302 | | 56.381 | 10.553 | 77.815 | 1.00 19.88 |
| | MOTA | | CB LEU B 302 | | 54.957 | 10.702 | 78.362 | 1.00 21.72 |
| | ATOM · | | G LEU B 302 | | 53.767 | 10.118 | 77.606 | |
| | ATOM | 5412 (| D1 LEU B 302 | | 52.576 | 9.980 | 78.549 | 1.00 31.08 |
| | ATOM | 5413 C | D2 LEU B 302 | | 53.434 | 11.011 | 76.415 | 1.00 31.35 |
| | ATOM | 5414 C | | | 56.445 | 10.988 | 76.351 | 1.00 27.11 |
| | ATOM | 5415 O | LEU B 302 | | 56.473 | 10.149 | 75.449 | 1.00 21.13 |
| | ATOM | 5416 N | | | 56.472 | 12.293 | 76.115 | 1.00 21.76 |
| | MOTA | 5417 C | | | 56.516 | 12.811 | | 1.00 17.69 |
| | ATOM | 5418 C | | | 56.357 | | 74.755 | 1.00 17.79 |
| | ATOM | 5419 C | | | 57.803 | 14.326 | 74.780 | 1.00 24.50 |
| | ATOM | 5420 O | | | | 12.425 | 74.040 | 1.00 20.84 |
| | MOTA | 5421 N | ARG B 304 | | 57.781 | 11.968 | 72.891 | 1,00 19.33 |
| | MOTA | 5422 C | | | 58.930 | 12.594 | 74.723 | 1.00 21.08 |
| | MOTA | 5423 CI | | | 60.215 | 12.269 | 74.120 | 1.00 25.56 |
| | MOTA | | 3 ARG B 304 | | 61.375 | 12.825 | 74.962 | 1.00 18.37 |
| | ATOM | | | | 61.427 | 14.356 | 75.072 | 1.00 23.12 |
| | | | | | 62.797 | 14.758 | 75.624 | 1.00 29.00 |
| | MOTA | 5426 NE | | | 63.073 | 13.938 | 76.789 | 1.00 33.28 |
| | MOTA | 5427 CZ | | | 64.271 | 13.689 | 77.283 | 1.00 30.24 |
| | MOTA | 5428 NH | 11 ARG B 304 | | 65.363 | 14.194 | 76.723 | 1.00 24.98 |
| | STOM | | 2 ARG B 304 | | 64.365 | 12.896 | 78.333 | |
| | MOTA | 5430 C | ARG B 304 | | 60.406 | 10.775 | 73.922 | 1.00 36.15 |
| ; | ATCM | 5431 0 | ARG B 304 | | 60.850 | 10.775 | | 1.00 20.46 |
| 2 | MOT | 5432 N | ALA B 305 | | 60.070 | | 72.868 | 1.00 18-70 |
| 3 | TOM . | 5433 CA | ALA B 305 | | 60.226 | 9.988 | 74.937 | 1.00 22.48 |
| | | 5434 CB | | | 59.847 | 8.542 | 74.845 | 1.00 19.70 |
| | | 5435 C | ALA B 305 | | | 7.894 | 76.174 | 1.00 24.24 |
| | | - 100 | | | 59.407 | 7.930 | 73.711 | 1.00 15.82 |
| | | | | | | - | • | |

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| MOTA | 5436 | 0 | ALA B | 305 | 59.938 | 7.184 | 72.888 | 1.00 | 19.12 |
|--------|------|-----|-------|-----|----------------|--------|--------|------|-------|
| | 5437 | N | TRP B | 306 | 58.113 | 8.230 | 73.659 | 1 00 | 18.65 |
| MOTA | | | | | | | | | |
| ATOM | 5438 | CA | TRP B | 306 | 57.298 | 7.668 | 72.600 | 1.00 | 19.57 |
| | 5439 | CB | TRP B | 306 | 55.800 | 7.856 | 72.893 | 1.00 | 18.26 |
| MOTA | | | | | | | | | |
| MOTA | 5440 | CG | TRP B | | 55.301 | 6.911 | 73.953 | | 20.71 |
| ATOM | 5441 | CD2 | TRP B | 306 | 54.087 | 7.025 | 74.708 | 1.00 | 23.94 |
| | | | | | | | 75.513 | | 24.73 |
| MOTY | 5442 | CE2 | TRP B | | 53.988 | 5.870 | | | |
| ATOM | 5443 | CE3 | TRP B | 306 | 53.073 | 7.991 | 74.780 | 1.00 | 26.01 |
| | | | | | 55.872 | 5.721 | 74.326 | 1 00 | 20.04 |
| MOTA | 5444 | CD1 | | | | | | | |
| ATOM | 5445 | NE1 | TRP B | 306 | 55.092 | 5.093 | 75.260 | 1.00 | 19.17 |
| | 5446 | CZ2 | | | 52.912 | 5.655 | 76.385 | 1.00 | 28.04 |
| ATOM | | | | | | | | | |
| MOTA | 5447 | CZ3 | TRP B | 306 | 52.001 | 7.779 | 75.646 | | 28.68 |
| MOTA | 5448 | CH2 | TRP B | 306 | 51.930 | 6.619 | 76.437 | 1.00 | 31.22 |
| | | | | | 57.665 | | 71.226 | | 23.48 |
| MOTA | 5449 | C | TRP B | | | 8.223 | | | |
| ATOM | 5450 | 0 | TRP B | 306 | 57.416 | 7.574 | 70.212 | 1.00 | 22.38 |
| | - | | THR B | | 58.262 | 9.412 | 71.176 | 1 00 | 22.36 |
| MOTA | 5451 | N | | | | | | | |
| ATOM | 5452 | CA | THR B | 307 | 58.672 | 9.953 | 69.880 | | 25.94 |
| ATOM | 5453 | CB | THR B | 307 | 59.143 | 11.417 | 69.986 | 1.00 | 25.88 |
| | | | | | | | | | 21.07 |
| ATOM | 5454 | 0G1 | THR B | 307 | 58.015 | 12.261 | 70.258 | | |
| ATOM | 5455 | CG2 | THR B | 307 | 59.827 | 11.864 | 68.686 | 1.00 | 22.52 |
| | | | THR B | | 59.815 | 9.078 | 69.350 | 1 00 | 30.09 |
| MOTA | 5456 | С | | | | | | | |
| ATOM | 5457 | 0 | THR B | 307 | 59.922 | 8.834 | 68.144 | 1.00 | 25.82 |
| ATOM | 5458 | N | LEU B | 308 | 60.664 | 8.596 | 70.258 | 1.00 | 27.54 |
| | | | | | | | | | 26.76 |
| MOTA | 5459 | CA | LEU B | 308 | 61.773 | 7.734 | 69.857 | | |
| ATOM | 5460 | CB | LEU B | 308 | 62.691 | 7.424 | 71.054 | 1.00 | 24.24 |
| | | | LEU B | | 63.420 | 8.614 | 71.718 | 1 00 | 31.16 |
| MOTA | 5461 | CG | | | | | | | |
| ATOM | 5462 | CD1 | LEU B | 308 | 64.282 | 8.147 | 72.877 | 1.00 | 24.71 |
| | 5463 | | LEU B | | 64.289 | 9.325 | 70.700 | 1.00 | 24.59 |
| ATOM | | | | | | | | | 27.20 |
| MOTA | 5464 | С | LEU B | 308 | 61.184 | 6.443 | 69.287 | | |
| ATOM | 5465 | 0 | LEU B | 308 | 61.609 | 5.961 | 68.234 | 1.60 | 23.52 |
| | | | ILE B | | 60.190 | 5.898 | 69.980 | 1 00 | 25.10 |
| ATOM | 5466 | Ŋ | | _ | | | | | |
| MOTA | 5467 | ÇA | ILE B | 309 | 59.53 7 | 4.679 | 69.530 | | 25.14 |
| ATOM | 5468 | CB | ILE B | 309 | 58.387 | 4.266 | 70.485 | 1.00 | 27.05 |
| | | | | | | 3.058 | 69.926 | 1 00 | 23.57 |
| MOTA | 5469 | CG2 | ILE B | | 57.646 | | | | |
| ATOM | 5470 | CG1 | ILE B | 309 | 58.952 | 3.947 | 71.868 | 1.00 | 22.98 |
| | 5471 | | ILE B | | 59.927 | 2.793 | 71.868 | 1.00 | 24.25 |
| MOTA | | | | | | | | | 25.41 |
| ATOM | 5472 | С | ILE B | 309 | 58.958 | 4.885 | 68.133 | | |
| ATOM | 5473 | 0 | ILE B | 309 | 59.177 | 4.064 | 67.243 | 1.00 | 22.13 |
| | | | | | 58.232 | 5.984 | 67.943 | 1 00 | 27.45 |
| MOTA | 5474 | N | TRP B | | | | | | |
| MOTA | 5475 | CA | TRP B | 310 | 57.618 | 6.266 | 66.548 | | 29.27 |
| ATOM | 5476 | CB | TRP B | 310 | 56.721 | 7.505 | 66.715 | 1.00 | 27.00 |
| | | | | | 56.112 | 7.847 | 65.378 | 3 00 | 28.26 |
| MOTA | 5477 | CG | TRP B | | | | | | |
| ATOM | 5478 | CD2 | TRP B | 310 | 55.172 | 7.061 | 64.633 | | 27.50 |
| | 5479 | CE2 | TRP B | | 54.947 | 7.729 | 63.408 | 1.00 | 30.47 |
| ATOM | | | | | | | 64.877 | | 29.85 |
| MOTA | 5480 | CE3 | TRP B | 310 | 54.500 | 5.856 | | | |
| MOTA | 5481 | CD1 | TRP B | 310 | 56.406 | ۶.929 | 64.597 | 1.00 | 29.76 |
| | | NE1 | | | 55.713 | 865 | 63.415 | 1.00 | 26.71 |
| MOTA | 5482 | | | | | | | | |
| MOTA | 5483 | CZ2 | TRP B | 310 | 54.076 | .234 | 62.429 | 1.00 | |
| ATOM | 5484 | CZ3 | TRP B | 310 | 53.636 | 5.362 | 63.901 | 1.00 | 30.24 |
| | | | | | | | 62.692 | 1 00 | 27.63 |
| ATOM | 5485 | CH2 | | | 53.433 | 6.053 | | | |
| ATOM | 5486 | С | TRP B | 310 | 58.629 | 6.424 | 65.520 | 1.00 | 30.16 |
| | | | TRP B | 210 | 58.378 | 5.964 | 64.410 | 1.00 | 30.04 |
| ATOM | 5487 | 0 | | | 50.570 | | | | 24.26 |
| ATOM | 5488 | N | CYS B | 311 | 59.762 | 7.069 | 65.793 | | |
| ATOM | 5489 | CA | CYS B | | 60.782 | 7.233 | 64.764 | 1.00 | 27.97 |
| | | | | | 61.893 | 8.157 | 65.252 | 1.00 | 28.21 |
| MOTA | 5490 | CB | CYS B | | | | | | |
| MOTA | 5491 | ŞG | CYS B | 311 | 61.422 | 9.905 | 65.381 | | 33.38 |
| | 5492 | c | CYS B | | 61.380 | 5.886 | 64.351 | 1.00 | 30.02 |
| ATOM | | | | | | | 63.172 | | 25.45 |
| MOTA | 5493 | 0 | CYS B | | 61.670 | 5.660 | | | |
| MOTA | 5494 | N | GLU B | 312 | 61.570 | 5.001 | 65.327 | | 31.59 |
| | | | | | 62.111 | 3.669 | 65.067 | 1.00 | 33.48 |
| MOTA | 5495 | CA | SLU B | | | | | | |
| ATOM | 5496 | CE | GLU B | 312 | 62.142 | 2.843 | 66.352 | | 34.78 |
| | | CG | GLU B | | 63.487 | 2.307 | 66.758 | 1.00 | 39.45 |
| ATOM | 5497 | | 300 0 | 214 | | | | | 40.11 |
| ATOM | 5498 | CD | GLU B | 312 | 64.171 | 1.513 | 65.675 | | |
| ATOM . | 5499 | OE! | GLU B | 312 | 63.539 | 0.614 | 65.081 | | 43.69 |
| | | 053 | GLU B | 312 | 65.358 | 1.782 | 65.437 | 1.00 | 39.26 |
| ATCM | 5500 | | ط بری | 244 | | | | | |
| ATCM | 5501 | С | GLU B | 212 | 61.197 | 2.959 | 64.080 | ±.00 | 29.97 |
| | | | | | | | | | |

| MOTA | 5502 | 2 0 | .GLU B 3 | 12 | 61.640 | 2.497 | 63.035 | 1.00 31.38 |
|------|-------|-----|-----------|----|------------------|-----------------|------------------|--------------------------|
| MOTA | 5503 | | | 13 | 59.919 | | | 1.00 31.38 |
| MOTA | 5504 | | | | 58.930 | | 63.598 | 1.00 26.73 |
| MOTA | 5505 | | | | 57.571 | | 64.297 | 1.00 25.83 |
| MOTA | 5506 | | | | 57.429 | | | |
| ATOM | 5507 | | 1 LEU B 3 | | 56.063 | | | 1.00 35.18 |
| ATOM | 550.8 | | 2 LEU B 3 | | 57.595 | | 66.130 64.989 | 1.00 32.49 |
| ATOM | 5509 | | LEU B 3 | _ | 58.768 | | | 1.00 29.71 |
| ATOM | 5510 | | LEU B 3 | | 58.716 | | | 1.00 29.03 |
| MOTA | 5511 | | SER B 3 | | 58.677 | | 61.228 | 1.00 25.39 |
| ATOM | 5512 | | | | 58.498 | | 62.263 | 1.00 30.13 |
| ATOM | 5513 | | | | 58.206 | | 61.060 | 1.00 34.06 |
| ATOM | 5514 | | | | 57.041 | | 61.445 | 1.00 31.15 |
| ATOM | 5515 | | SER B 31 | | 59.707 | | 62.234 | 1.00 48.58 |
| ATOM | 5516 | | SER B 31 | | 59.632 | | 60.151 | 1.00 31.84 |
| ATOM | 5517 | | GLY B 31 | | 60.831 | 5.469 4.515 | 59.026 | 1.00 34.15 |
| ATOM | 5518 | | | | 62.036 | | 60.655 | 1.00 31.81 |
| ATOM | 5519 | | GLY B 31 | | 62.659 | 4.485 | 59.848 | 1.00 37.27 |
| ATOM | 5520 | | GLY B 31 | | | 5.851 | 59.616 | 1.00 39.93 |
| MOTA | 5521 | N | ARG B 31 | | 63.363 | 6.054 | 58.624 | 1.00 39.79 |
| MOTA | 5522 | CA | ARG B 31 | | 62.422 | 6.798 | 60.518 | 1.00 38.22 |
| ATOM | 5523 | CB | ARG B 31 | | 63.004 | 8.121 | 60.336 | 1.00 38.66 |
| ATOM | 5524 | CG | ARG B 31 | | 61.908 61.089 | 9.184 | 60.275 | 1.00 40.20 |
| MOTA | 5525 | CD | ARG B 31 | | | 9.345 | 61.520 | 1.00 39.06 |
| ATOM | 5526 | NE | ARG B 31 | | | 10.398 | 61.284 | 1.00 42.13 |
| ATOM | 5527 | CZ | ARG B 31 | | 59.002 | 9.954 | 60.352 | 1.00 45.09 |
| MOTA | 5528 | NH: | | | 58.075 | 10.754 | 59.838 | 1.00 40.84 |
| ATOM | 5529 | NH | | | 58.064 57.150 | 12.033 | 60.170 | 1.00 48.44 |
| ATOM | 5530 | C | ARG B 31 | | 64.031 | 10.278 8.467 | 59.014 | 1.00 35.96 |
| ATOM | 5531 | ō | ARG B 31 | | 63.952 | 7.988 | 61.408 | 1.00 39.03 |
| ATOM | 5532 | N | GLU-B 31 | | 65.003 | 9.296 | 62.539 61.035 | 1.00 34.34 |
| ATOM | 5533 | CA | GLU B 31 | | 66.074 | 9.697 | 61.943 | 1.00 39.58 1.00 43.35 |
| ATOM | 5534 | CB | GLU B 31 | | 67.142 | 10.509 | 61.203 | 1.00 49.34 |
| ATOM | 5535 | CG | GLU B 31 | | 67.609 | 9.910 | 59.884 | 1.00 49.34 |
| ATOM | 5536 | CD | GLU B 31 | | 66.546 | 10.009 | 58.798 | 1.00 57.04 |
| ATOM | 5537 | OE1 | | | 66.146 | 11.149 | 58.467 | 1.00 63.46 |
| ATOM | 5538 | OE2 | | | 66.108 | 8.954 | 58.280 | 1.00 64.46 |
| MOTA | 5539 | С | GLU B 31 | | 65.555 | 10.528 | 63.100 | 1.00 41.58 |
| ATOM | 5540 | 0 | GLU B 31 | | 64.658 | 11.356 | 62.939 | 1.00 39.74 |
| MOTA | 5541 | N | VAL B 318 | 3 | 66.118 | 10.301 | 64.278 | 1.00 35.38 |
| ATOM | 5542 | CA | VAL B 318 | | 65.706 | 11.049 | 65.448 | 1.00 38.76 |
| MOTA | 5543 | CB | VAL B 318 | 3 | 66.000 | 10.265 | 66.750 | 1.00 42.28 |
| MOTA | 5544 | CG1 | VAL B 318 | 3 | 65.560 | 11.080 | 67.962 | 1.00 38.26 |
| MOTA | 5545 | CG2 | VAL B 318 | 3 | 65.287 | 8.916 | 66.722 | 1.00 39.99 |
| ATOM | 5546 | С | VAL B 318 | 3 | 66.459 | 12.370 | 65.478 | 1.00 41.82 |
| .TOM | 5547 | 0 | VAL B 318 | 3 | 67.689 | 12.395. | 65.570 | 1.00 37.20 |
| ATOM | 5548 | N | PRO B 319 |) | 65.735 | 13.491 | 65.356 | 1.00 43.18 |
| ATOM | 5549 | CD | PRO B 319 |) | 64.290 | 13.672 | 65.155 | 1.00 41.90 |
| MOTA | 5550 | CA | PRO B 319 | | 66.402 | 14.792 | 65.388 | 1.00 44.31 |
| MOTA | 5551 | CB | PRO B 319 | | 65.241 | 15.763 | 65.181 | 1.00 44.58 |
| ATOM | 5552 | CG | PRO B 319 | | 64.079 | 15.011 | 65.795 | 1.00 43.34 |
| ATOM | 5553 | C | PRO B 319 | | 67.086 | 14.965 | 66.741 | 1.00 44.62 |
| ATOM | 5554 | o | PRO B 319 | | 66.541 | 14.565 | 67.771 | 1.00 43.75 |
| ATOM | .5555 | N | GLU B 320 | | 68.277 | 15.552 | 66.735 | 1.00 44.16 |
| MOTA | 5556 | CA | GLU B 320 | | 69.029 | 15.762 | 67.967 | 1.00 45.92 |
| MOTA | 5557 | CB | GLU B 320 | | 70.381 | 16.406 | 67.663 | 1.00 50.87 |
| MOTA | 5558 | CG | GLU B 320 | | 71.165 | 16.768 | 68.919 | 1.00 53.71 |
| MOTA | 5559 | CD | GLU B 320 | | 72.455 | 17.505 | 68.620 | 1.00 57.75 |
| MOTA | 5560 | OE1 | GLU B 320 | | 73.161 | 17.874 | 69.583 | 1.00 56.37 |
| MOTA | 5561 | 0E2 | GLU B 320 | | 72.762 | 17.714 | 67.427 | 1.00 60.07 |
| ATOM | 5562 | C | GLU B 320 | | 68.311 | 16.625 | 68.995 | 1.00 44,42 |
| MOTA | 5563 | 0 | GLU B 320 | | 68.244 | 16.279 | 70.168 | 1.00 42.32 |
| ATOM | 5564 | N | LYS B 321 | - | 67.778 | 17.753 | 68.550 | 1.00 42.50 |
| MOTA | 5565 | CA | LYS B 321 | | 67.102 | 18.672 | 69.448 | 1.00 45.24 |
| MOTA | 5566 | CB | LYS B 321 | | 67.853 | 20.000 | 69.503 | 1.00 46.43 |
| HOTA | 5567 | CG | LYS B 321 | | 67.890 | 20.802 | 68.195 | 1.00 51.45 |
| | | | | | | | | |

| ATOM | 5568 | CD | LYS B | 321 | | 68.700 | 20.144 | 67.057 | 1.00 | |
|------|------|-----|--------|-----|-------|--------|----------------|--------|--------|---------|
| | | CE | LYS B | | | 67.936 | 19.062 | 66.280 | 1.00 5 | 55.24 |
| ATOM | 5569 | | | | | 66.738 | 19.588 | 65.558 | 1.00 | 55.31 |
| ATOM | 5570 | NZ | LYS B | | | | 18.971 | 69.098 | 1.00 | |
| MOTA | 5571 | С | | 321 | | 65.662 | | 67.978 | 1.00 | • |
| ATOM | 5572 | 0 | LYS B | 321 | | 65.211 | 18.736 | | | |
| ATOM | 5573 | N | LEU B | 322 | | 64.947 | 19.512 | 70.076 | | 39.45 |
| ATOM | 5574 | CA | LEU B | 322 | | 63.563 | 19.885 | 69.875 | 1.00 | |
| | 5575 | CB | | 322 | | 62.846 | 20.034 | 71.215 | 1.00 | 40.88 |
| ATOM | | | | 322 | | 62.943 | 18.901 | 72.234 | 1.00 | 40.09 |
| MOTA | 5576 | CG | | | | 62.001 | 19.175 | 73.388 | 1.00 | 38.17 |
| ATOM | 5577 | | LEU B | 322 | | | | 71.580 | 1.00 | 41 -56 |
| ATOM | 5578 | CD2 | | 322 | | 62.588 | 17.596 | 69.197 | 1.00 | A1 23 |
| ATOM | 5579 | С | LEU B | 322 | | 63.615 | 21.244 | | 1.00 | 30.33 |
| ATOM | 5580 | 0 | LEU B | 322 | • | 64.466 | 22.070 | 69.531 | 1.00 | |
| ATOM | 5581 | N | ASN B | 323 | | 62.735 | 21.473 | 68.233 | 1.00 | |
| | 5582 | CA | ASN B | | | 62.703 | 22.771 | 67.582 | 1.00 | |
| MOTA | | CB | ASN B | | | 61.985 | 22.707 | 66.234 | 1.00 | 41.53 |
| MOTA | 5583 | | ASN B | | | 60.617 | 22.085 | 66.335 | 1.00 | 41.89 |
| MOTA | 5584 | CG | | | | | 22.308 | 67.304 | | 39.79 |
| ATOM | 5585 | | | 323 | | 59.889 | 21.317 | 65.317 | | 40.43 |
| MOTA | 5586 | ND2 | ASN B | | | 60.243 | | | | 44.76 |
| MOTA | 5587 | С | ASN B | 323 | | 61.949 | 23.690 | 68.532 | | |
| ATOM | 5588 | 0 | ASN B | 323 | | 61.402 | 23.237 | 69.539 | | 45.80 |
| ATOM | 5589 | N | ASN B | 324 | | 61.902 | 24.973 | 68.210 | 1.00 | 46.85 |
| | 5590 | CA | ASN B | | | 61.234 | 25.930 | 69.076 | 1.00 | 47.60 |
| MOTA | 5591 | CB | ASN B | | | 61.460 | 27.348 | 68.549 | 1.00 | 50.87 |
| ATOM | | | ASN B | | | 61.089 | 28.407 | 69.562 | 1.00 | 55.06 |
| ATOM | 5592 | CG | | | | 59.925 | 28.565 | 69.919 | 1.00 | 60.68 |
| atom | 5593 | | ASN B | | | 62.091 | 29.131 | 70.048 | 1.00 | 59.17 |
| ATOM | 5594 | ND2 | :ASN B | | | 02.091 | 25.664 | 69.249 | | 43.97 |
| ATOM | 5595 | С | ASN B | | | 59.740 | | 70.322 | | 41.33 |
| ATOM | 5596 | 0 | ASN B | 324 | | 59.190 | 25.898 | | | 43.49 |
| ATOM | 5597 | N | LYS B | 325 | | 59.087 | 25.168 | 68.201 | | |
| ATOM | 5598 | CA | LYS B | 325 | | 57.655 | 24.892 | 68.264 | | 45.95 |
| | 5599 | CB | LYS B | | | 57.112 | 24.415 | 66.909 | 1.00 | |
| ATOM | 5600 | CG | LYS B | | | 57,212 | 25.400 | 65.731 | | 53.41 |
| ATOM | | CD | LYS B | | | 58.582 | 25.386 | 65.024 | | 58.77 |
| MOTA | 5601 | | | | | 59.700 | 26.013 | 65.846 | 1.00 | 58.10 |
| MOTA | 5602 | CE | LYS B | | | 61.024 | 25.906 | 65.178 | | 53.38 |
| ATOM | 5603 | NZ | LYS B | | | | 23.822 | 69.309 | | 45.79 |
| ATOM | 5604 | С | LYS B | | | 57.368 | | 70.034 | | 43.91 |
| ATOM | 5605 | 0 | LYS B | | | 56.375 | 23.891 | | | 44.28 |
| ATOM | 5606 | N | ALA B | 326 | | 58.245 | 22.829 | 69.381 | | 44.25 |
| ATOM | 5607 | CA | ALA B | 326 | | 58.078 | 21.746 | 70.336 | | |
| ATOM | 5608 | CB | ALA B | 326 | | 59.013 | 20.589 | 69.986 | | 41.44 |
| | 5609 | c | ALA B | | | 58.342 | 22.233 | 71.757 | | 40.92 |
| ATOM | 5610 | ō | ALA B | | | 57.639 | 21.843 | 72.688 | | 39.02 |
| ATOM | | | LYS B | | | 59.352 | 23.085 | 71.922 | | 38.14 |
| ATOM | 5611 | N | | | | 59.689 | 23.603 | 73.246 | 1.00 | 40.11 |
| ATOM | 5612 | CA | LYS B | | | | 24.552 | 73.178 | 1.00 | |
| ATCM | 5613 | СВ | LYS B | | | 60.892 | | 72.(59 | | 45.78 |
| ATOM | 5614 | CG | LYS B | | | 62.174 | 23.922 | 72.675 | | 48.46 |
| ATOM | 5615 | CD | LYS B | | | 63.325 | 24.926 | | | 49.62 |
| ATOM | 5616 | CE | LYS B | 327 | | 64.594 | 24.367 | 72.031 | | |
| ATOM | 5617 | NZ | LYS B | 327 | | 65.108 | 23.139 | 72.700 | | 48.53 |
| | 5618 | С | LYS B | 327 | | 58.500 | 24.338 | 73.841 | | 39.17 |
| MOTA | | ō | LYS B | | | 58.132 | 2 4.112 | 74.994 | 1.00 | 38.87 |
| ATOM | 5619 | | | | | 57.898 | 25.215 | 73.048 | 1.00 | 41.06 |
| ATOM | 5620 | N | GLU B | | | 56.750 | 25.986 | 73.512 | | 42.35 |
| MOTA | 5621 | CA | GLU B | | | | 27.028 | 72.463 | | 44.02 |
| ATOM | 5622 | CB | GLU B | | | 56.357 | | 72.258 | | 44.80 |
| ATOM | 5623 | CG | GLU B | | | 57.434 | 28.084 | | | 48.40 |
| TOM | 5624 | CD | GLU B | 328 | | 57.835 | 28.742 | 73.569 | 1.00 | 5 30.30 |
| ATOM | 5625 | OE1 | GLU B | 328 | | 56.949 | 29.317 | 74.237 | 1.00 | 51.20 |
| | 5626 | | GLU B | | | 59.029 | 28.680 | 73.935 | | 47.81 |
| ATOM | | C | GLU B | | | 55.569 | 25.087 | 73.839 | | 38.67 |
| ATOM | 5627 | | GLU B | | | 54.794 | 25.377 | 74.750 | 1.00 | 41.20 |
| atom | 5628 | 0 | | _ | | 55.429 | 23.999 | 73.090 | | 35.31 |
| ATCM | 5629 | N | LEU B | | | | 23.056 | 73.334 | | 32.69 |
| ATCM | 5630 | CA | LEU B | | | 54.349 | 23.000 | | | 35.06 |
| ATOM | 5631 | CB | LEU E | 329 | | 54.404 | 21.900 | | | 35.01 |
| ATOM | 5632 | CG | LEU E | 329 | | 53.344 | 20.813 | 72.544 | | |
| | 5633 | | LEU E | | | 51.958 | 21.430 | 72.419 | 1.00 | 36.90 |
| ATOM | | | | | | | | | | |
| | | | | | RECON | | | | | |

| ATOM | | 53.52 | 1 19.69 | 9 71.525 | 1.00 32.36 |
|--------------|--|------------------|----------------------|--------------------------|--------------------------|
| ATOM | | 54.50 | 4 22.50 | | |
| ATOM ATOM | 0 0 0 , DD0 D 343 | 53.62 | _ | | 1.00 30.53 |
| ATOM | == == == == == = = = = = = = = = = | 55.64 | 0 21.87 | | 1.00 32.74 |
| ATOM | | 55.88 57.26 | 9 21.31 | | |
| ATOM | | 57.46 | 7 20.642 6 19.428 | | |
| ATOM | | 58.83 | 2 18.81 | | 1.00 34.91 |
| ATOM | | 56.36 | 9 18.396 | | 1.00 34.10 |
| ATOM ATOM | | 55.789 | | 3 77.429 | 1.00 37.12 |
| ATOM | | 55.210 | | | |
| ATOM | | 56.353 56.313 | | - | |
| ATOM | 5647 CB LYS B 331 | 57.162 | | | |
| ATOM | 5648 CG LYS B 331 | 58.658 | | | 1.00 51.07 |
| ATOM ATOM | 5649 CD LYS B 331 | 59.482 | | 77.021 | 1.00 49.96 |
| ATOM | 5650 CE LYS B 331 5651 NZ LYS B 331 | 59.371 | | | 1.00 53.08 |
| ATOM | 5652 C LYS B 331 | 58.013 54.892 | 28.569 25.069 | | 1.00 56.18 |
| ATOM | 5653 O LYS B 331 | 54.588 | | | 1.00 42.06 1.00 43.05 |
| MOTA | 5654 N SER B 332 | 54.018 | | | 1.00 44.54 |
| MOTA | 5655 CA SER B 332 | 52.639 | | 77.679 | 1.00 46.58 |
| ATOM | 5656 CB SER B 332 5657 OG SER B 332 | 51.975 | | | 1.00 48.75 |
| ATOM | 5658 C SER B 332 | 51.769 51.780 | | ,- | 1.00 49.55 |
| ATOM | 5659 O SER B 332 | 50.618 | | | 1.00 49.56 1.00 46.67 |
| ATOM | 5660 N ILE B 333 | 52.341 | | | 1.00 50.55 |
| ATOM | 5661 CA ILE B 333 | 51.586 | | | 1.00 51.93 |
| ATOM ATOM | 5662 CB ILE B 333 5663 CG2 ILE B 333 | 52.259 | 20.945 | 79.376 | 1.00 51.82 |
| ATOM | 5664 CG1 ILE B 333 | 51.447 52.359 | 19.902 20.539 | 80.134 77.905 | 1.00 50.29 |
| ATOM | 5665 CD1 ILE B 333 | 53.044 | 19.210 | 77.693 | 1.00 52.18 1.00 55.42 |
| ATOM | 5666 C ILE B 333 | 51.367 | 22.634 | 80.964 | 1.00 51.45 |
| MOTA | 5667 O ILE B 333. | 52.180 | 23.290 | 81.614 | 1.00 50.96 |
| ATOM ATOM | 5668 N ASP B 334 5669 CA ASP B 334 | 50.245 | 22.141 | 81.472 | 1.00 54.05 |
| ATOM | 5670 CB ASP B 334 | 49.850 48.320 | 22.306 22.216 | 82.865 | 1.00 58.15 |
| ATOM | . 5671 CG ASP B 334 | 47.751 | 20.972 | 82.959 82.262 | 1.00 60.38 1.00 63.85 |
| ATOM | 5672 OD1 ASP B 334 | 48.017 | 19.833 | 82.710 | 1.00 59.16 |
| ATOM ATOM | 5673 OD2 ASP B 334 5674 C ASP B 334 | 47.033 | 21.138 | 81.252 | 1.00 59.71 |
| ATOM | 5674 C ASP B 334 5675 O ASP B 334 | 50.506 | 21.207 | 83.701 | 1.00 55.47 |
| ATOM | 5676 N PHE B 335 | 49.833 51.816 | 20.291 21.307 | 84.171 83.906 | 1.00 54.08 1.00 54.60 |
| MOTA | 5677 CA PHE B 335 | 52.524 | 20.266 | 84.641 | 1.00 54.60 1.00 56.60 |
| ATOM | 5678 CB PHE B 335 | 53.718 | 19.784 | 83.811 | 1.00 53.01 |
| MOTA MOTA | 5679 CG PHE B 335 5686 CD1 PHE B 335 | 54.522 | | 84.482 | 1.00 49.30 |
| ATOM | 5681 CD2 PHE B 335 | 53.898 55.901 | 17.589 18.843 | 85.008 | 1.00 45.61 |
| ATOM | 5682 CE1 PHE B 335 | 54.637 | 16.600 | 84.605 85.651 | 1.00 46.83 1.00 45.95 |
| MOTA | 5683 CE2 PHE B 335 | 56.651 | 17.860 | 85.247 | 1.00 45.93 |
| MOTA | 5684 CZ PHE B 335 | 56.018 | 16.737 | 85.772 | 1.00 46.08 |
| ATOM ATOM | 5685 C PHE B 335 5686 O PHE B 335 | 52.971 | 20.559 | 86.072 | 1.00 57.29 |
| ATOM | 5686 O PHE B 335 5687 N GLU B 336 | 52.197 54.223 | 20.378 20.983 | 87.012 | 1.00 63.54 |
| MOTA | 5688 CA GLU B 336 | 54.818 | 20.983 | 86.229 87.535 | 1.00 55.21 1.00 60.30 |
| MOTA | 5689 CB GLU B 336 | 53.783 | 21.846 | 88.517 | 1.00 64.95 |
| ATOM | 5690 CG GLU B 336 | 54.375 | 22.225 | 89.867 | 1.00 71.50 |
| ATOM ATOM | 5691 CD GLU B 336 5692 OE1 GLU B 336 | 53.363 | 22.882 | 90.787 | 1.00 75.37 |
| ATOM | 5692 OE1 GLU B 336 5693 OE2 GLU B 336 | 52.796 53.137 | 23.925 | 90.394 | 1.00 75.32 |
| MOTA | 5694 C GLU B 336 | 55.485 | 22.361 20.058 | 91.9 01 88.146 | 1.00 76.84 1.00 55.66 |
| ATOM | 5695 O GLU B 336 | 54.823 | 19.093 | 88.529 | 1.00 35.66 |
| MOTA | 5696 N GLU B 337 | 56.807 | 20.125 | 88.240 | 1.00 54.26 |
| ATCH ATCH | 5697 CA GLU B 337 | 57.630 | 19.047 | 88.767 | 1.00 54.35 |
| ATOM | 5698 CB GLU B 337 5699 CG GLU B 337 | 59.101 | 19.457 | 88.635 | 1.00 54.08 |
| | | 60.074 | 18.315 | 88.514 | 1.00 54.15 |

PCT/US00/24700

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| | | | • | | | | | |
|--------|---------------|-------|---------|------------|--------|--------|--------|---------------------|
| ATOM | 5700 | CD | GLU B | 337 | 59.856 | 17.496 | 87.259 | 1.00 48.94 |
| | | | | | | | | |
| MOTA | 5701 | OE: | _ | | 59.958 | 18.049 | 86.142 | 1.00 41.06 |
| ATOM | 5702 | 0E2 | GLU B | 337 | 59.581 | 16.292 | 87.391 | 1.00 50.23 |
| ATOM | 5703 | С | GLU B | 337 | 57.278 | 18.740 | 90.227 | 1.00 55.08 |
| | 5704 | ō | GLU B | | 57.130 | 19.651 | 91.039 | 1.00 54.51 |
| ATOM | | | | | | | | |
| ATOM | 5705 | N | PHE B | | 57.140 | 17.458 | 90.557 | 1.00 56.20 |
| MOTA | 5706 | CA | PHE B | 338 | 56.798 | 17.048 | 91.918 | 1.00 57.73 |
| MOTA | 5707 | CB | PHE B | 338 | 56.713 | 15.527 | 92.020 | 1.00 58.47 |
| | | | PHE B | | 56.231 | 15.034 | 93.359 | 1.00 63.17 |
| ATOM | 5708 | CG | | | | | | |
| MOTA | 5709 | CDI | . PHE B | | 54.882 | 15.096 | 93.696 | 1.00 64.86 |
| ATOM | 5710 | CD2 | PHE B | 338 | 57.129 | 14.526 | 94.293 | 1.00 63.51 |
| ATOM | 5711 | CE1 | PHE B | 338 | 54.434 | 14.656 | 94.943 | 1.00 65.25 |
| | 5712 | CE2 | | | 56.693 | 14.087 | 95.539 | 1.00 63.64 |
| MOTA | | | | | | | | |
| ATOM | 5713 | CZ | PHE B | | 55.342 | 14.152 | 95.864 | 1.00 66.30 |
| MOTA | 5714 | С | PHE B | 338 | 57.836 | 17.539 | 92.918 | 1.00 61.85 |
| ATOM | 5715 | 0 | PHE B | 338 | 57.520 | 17.807 | 94.078 | 1.00 58 <i>.</i> 15 |
| MOTA | 5716 | N | ASP B | | 59.081 | 17.636 | 92.466 | 1.00 64.63 |
| | | | | | | | 93.316 | 1.00 67.53 |
| MOTA | 5717 | CA | ASP B | | 60.167 | 18.099 | | |
| ATOM | 5718 | CB | ASP B | | 61.286 | 17.059 | 93.362 | 1.00 67.32 |
| ATOM · | 5719 | CG | ASP B | 339 | 62.474 | 17.524 | 94.174 | 1.00 68.13 |
| ATOM | 5720 | . OD1 | ASP B | | 62.280 | 17.909 | 95.346 | 1.00 68.68 |
| | 5721 | | ASP B | | 63.603 | 17.502 | 93.646 | 1.00 69.03 |
| MOTA | | | | | | | | |
| ATOM | 5722 | С | ASP B | | 60.718 | 19.435 | 92.829 | 1.00 69.03 |
| ATOM | 5723 | 0 | ASP B | 339 | 61.211 | 19.545 | 91.708 | 1.00 67.54 |
| ATOM | 5724 | N | ASP B | 340 | 60.626 | 20.442 | 93.693 | 1.00 72.19 |
| ATOM | 5725 | CA | ASP B | | 61.088 | 21.797 | 93.402 | 1.00 75.20 |
| | | | | | 61.113 | 22.623 | 94.689 | 1.00 77.04 |
| ATOM | 5726 | CB | ASP B | | | | | |
| A'TOM | 5727 | CG | ASP B | | 59.766 | 22.671 | 95.375 | 1.00 78.70 |
| ATOM | 5728 | OD1 | ASP B | 340 | 58.803 | 23.181 | 94.763 | 1.00 79.66 |
| ATOM | 5729 | OD2 | ASP B | 340 | 59.668 | 22.194 | 96.525 | 1.00 80.53 |
| ATOM | 5730 | C | ASP B | | 62.464 | 21.856 | 92.751 | 1.00 74.82 |
| | | | | | | 22.400 | 91.659 | 1.00 78.48 |
| ATOM | 5731 | 0 | ASP B | | 62.615 | | | |
| ATOM | 5732 | N | GLU B | | 63.465 | 21.303 | 93.426 | 1.00 74.11 |
| ATOM | 57 33 | CA | GLU B | 341 | 64.827 | 21.312 | 92.907 | 1.00 76.25 |
| ATOM | 5734 | CB | GLU B | 341 | 65.818 | 21.596 | 94.040 | 1.00 79.54 |
| | 5735 | CG | GLU B | | 67.277 | 21.653 | 93.596 | 1.00 82.33 |
| ATOM | | | | | | | 92.577 | 1.00 83.24 |
| ATOM | 5736 | CD | GLU B | | 67.539 | 22.750 | | |
| ATOM | 5 73 7 | OE1 | GLU B | 341 | 67.333 | 23.937 | 92.910 | 1.00 85.25 |
| MOTA | 5738 | OE2 | GLU B | 341 | 67.950 | 22.427 | 91.443 | 1.00 83.72 |
| ATOM | 5739 | С | GLU B | 341 | 65.196 | 19.998 | 92.227 | 1.00 73.97 |
| | 5740 | ō | GLU B | | 65.627 | 19.051 | 92.883 | 1.00 77.10 |
| ATOM | | | | | | | 90.910 | 1.00 71.92 |
| MOTA | 5741 | N | VAL B | | 65.033 | 19.946 | | |
| MOTA | 5742 | CA | VAL B | | 65.354 | 18.744 | 90.151 | 1.00 68.51 |
| ATOM | 5743 | CB | VAL B | 342 | 64.081 | 18.027 | 89.663 | 1.00 68.83 |
| ATOM | 5744 | CG1 | VAL B | 342 | 63.268 | 17.552 | 90.837 | 1.00 67.57 |
| | 5745 | | VAL B | | 63.255 | 18.969 | 88.806 | 1.00 67.72 |
| ATOM | | | | | 66.201 | 19.059 | 88.927 | 1.00 65 35 |
| ATOM | 5746 | C | VAL B | | | | | |
| ATOM | 5747 | 0 | VAL B | | 67.177 | 18.366 | 88.640 | 1.00 68.31 |
| MOTA | 5748 | N | ASP'B | 343 | 65.819 | 20.112 | 88.213 | 1.00 60.89 |
| ATOM | 5749 | CA | ASP B | 343 | 66.514 | 20.520 | 86.998 | 1.00 58.89 |
| | 5750 | CB | ASP B | | 68.024 | 20.636 | 87.223 | 1.00 63.48 |
| MOTA | | | | | | | 85.966 | 1.00 66.69 |
| ATOM | 5751 | CG | ASP B | | 68.763 | 21.070 | | |
| ATOM | 5752 | OD1 | ASP B | 343 | 70.012 | 21.070 | 85.970 | 1.00 67.64 |
| ATOM | 5753 | OD2 | ASP B | 343 | 68.089 | 21.420 | 84.973 | 1.00 65.42 |
| ATOM | 5754 | C | ASP B | | 66.264 | 19.499 | 85.900 | 1.00 53.17 |
| | | | | | 66.993 | 18.516 | 85.766 | 1.00 49.70 |
| ATOM | 5755 | 0 | ASP B | | | | | |
| ATOM | 5756 | N | ARG B | | 65.216 | 19.735 | 85.124 | 1.00 50.24 |
| MOTA | 5757 | CA | ARG B | 344 | 64.868 | 18.853 | 84.022 | 1.00 46.49 |
| ATOM | 5758 | CB | ARG B | | 63.467 | 18.269 | 84.228 | 1.00 42.41 |
| | | CG | ARG B | | 63.317 | 17.367 | 85.452 | 1.00 38.59 |
| MOTA | 5759 | | | | | 16.246 | 85.432 | 1.00 37.12 |
| ATOM | 5760 | CD | ARG B | | 64.344 | | | |
| ATOM | 5761 | NE | ARG B | | 64.169 | 15.310 | 86.537 | 1.00 -36.55 |
| ATOM | 5762 | CZ | ARG B | 344 | 65.078 | 14.413 | 86.905 | 1.00 37.20 |
| ATOM . | 5763 | | ARG B | | 66.234 | 14.331 | 86.259 | 1.00 33.53 |
| | | | ARG B | | 64.830 | 13.595 | 87.915 | 1.00 28.79 |
| MOTA | 5764 | | | | | | 82.732 | 1.00 44.45 |
| ATOM | 5765 | С | ARG B | 344 | 64.910 | 19.660 | 20.72 | T.00 44.43 |

| ATOM | | | 1 | 64.328 | 19.269 | 81.720 | 1.00 38.73 |
|--------------|--------------|------------------------------|---|------------------|------------------|------------------|--------------------------|
| ATOM | 576 | 7 N SER B 34. | 5 | 65.618 | | | |
| ATOM | | | 5 | 65.740 | | | |
| ATOM | | | | 66.661 | | | |
| ATOM | | | j | 67.956 | 22.388 | 82.351 | |
| ATOM | | | | 66.244 | | | |
| ALOW | 5772 | | | 65.840 | 21.333 | 79.273 | |
| ATOM | 5773 | | | 67.117 | 19.992 | 80.534 | |
| MOTA | 5774 | | | 67.661 | | 79.391 | |
| ATOM | 5775 | | | 68.660 | | 79.877 | 1.00 36.09 |
| MOTA | 5776 | | | 68.054 | | | 1.00 34.27 |
| MOTA MOTA | 5777 5778 | | | 67.433 | 16.013 | | |
| ATOM | 5779 | | | 66.843 | 15.048 | | |
| MOTA | 5780 | | | 68.072 | 17.294 | 82.157 | |
| ATOM | 5781 | | | 67.489 | 16.344 | 82.999 | |
| ATOM | 5782 | | | 66.878 66.310 | 15.228 | 82.457 | |
| ATOM | 5783 | | | 66.563 | 14.306 | 83.306 | 1.00 33.35 |
| ATOM | 5784 | | | .66.719 | 18.599 18.385 | 78.570 | 1.00 36.26 |
| ATOM | 5785 | N MET B 347 | | 65.445 | 18.282 | 77.367 79.214 | 1.00 40.50 |
| MOTA | 5786 | CA MET B 347 | | 64.346 | 17.628 | 78.516 | 1.00 32.72 1.00 35.43 |
| ATOM | 5787 | CB MET B 347 | | 63.280 | 17.164 | 79.513 | 1.00 34.36 |
| MOŢA | 5788 | CG MET B 347 | | 63.819 | 16.292 | 80.635 | 1.00 28.32 |
| ATOM | 5789 | SD MET B 347 | | 62.515 | 15.604 | 81.669 | 1.00 20.32 |
| ATOM | 5790 | CE MET B 347 | | 61.654 | 17.027 | 82.142 | 1.00 39.60 |
| MOTA | 5791 | C MET B 347 | | 63.701 | 18.525 | 77.465 | 1.00 39.04 |
| ATOM | 5792 | O MET B 347 | | 63.060 | 18.029 | 76.540 | 1.00 37.38 |
| ATOM | 5793 | N LEU B 348 | | 63.857 | 19.839 | 77.606 | 1.00 39.21 |
| MOTA MOTA | 5794 5795 | CA LEU B 348 | | 63.272 | 20.773 | 76.645 | 1.00 40.81 |
| ATOM | 5796 | CB LEU B 348 CG LEU B 348 | | 62.806 | 22.058 | 77.339 | 1.00 36.87 |
| MOTA | 5797 | CD1 LEU B 348 | | 61.690 | 21.975 | 78.384 | 1.00 42.66 |
| ATOM | 5798 | CD2 LEU B 348 | | 61.507 | 23.337 | 79.032 | 1.00 43.41 |
| ATOM | 5799 | C LEU B 348 | | 60.391 64.289 | 21.511 21,133 | 77.741 | 1.00 40.47 |
| ATOM | 5800 | O LEU B 348 | | 64.018 | 21,133 | 75.573 | 1.00 41.13 |
| ATOM | 5801 | N GLU B 349 | | 65.455 | 20.495 | 74.711 75.632 | 1.00 38.93 |
| ATOM | 5802 | CA GLU B 349 | | 66.527 | 20.757 | 74.681 | 1.00 37.70 1.00 42.48 |
| MOTA. | 5803 | CB GLU B 349 | | 67.856 | 20.953 | 75.422 | 1.00 45.02 |
| MOTA | 5804 | CG GLU B 349 | | 67.834 | 22.035 | 76.493 | 1.00 53.82 |
| MOTA | 5805 | CD GLU B 349 | | 67.483 | 23.402 | 75.938 | 1.00 57.46 |
| ATOM | 5806 | OE1 GLU B 349 | | 68.211 | 23.885 | 75.044 | 1.00 59.62 |
| ATOM | 5807 | OE2 GLU B 349 | | 66.480 | 23.993 | 76.397 | 1.00 57.91 |
| MOTA | 5808 | C GLU B 349 | | 66.709 | 19.638 | 73.664 | 1.00 43.57 |
| MOTA MOTA | 5809 5810 | O GLU B 349 N THR B 350 | | 66.577 | 19.849 | 72.459 | 1.00 41.26 |
| ATOM | 5811 | N THR B 350 CA THR B 350 | | 67.027 | 18.448 | 74.161 | 1.00 41.95 |
| ATOM | 5812 | CE THR B 350 | | 67.264 68.689 | 17.299 | 73.298 | 1.00 40.02 |
| ATOM | 5813 | OG1 THR B 350 | | 68.894 | 16.775 | 73.504 | 1.00 43.08 |
| ATOM . | | CG2 THR B 350 | | 69.703 | 16.490 17.816 | 74.894 73.049 | 1.00 41.07 1.00 45.05 |
| ATOM | 5815 | C THR B 350 | | 66.278 | 16.154 | 73.510 | 1.00 45.05 |
| ATOM | 5816 | O THR B 350 | | 65.754 | | 74.611 | 1.00 37.36 |
| MOTA | 5817 | N LEU B 351 | | 66.043 | 15.391 | 72.445 | 1.00 32.86 |
| MOTA | 5818 | CA LEU B 351 | | 65.126 | 14.260 | 72.475 | 1.00 35.00 |
| ATOM | 5819 | CB LEU B 351 | | 64.776 | 13.810 | 71.053 | 1.00 31.61 |
| MOTA | 5820 | CG LEU B 351 | | 63.709 | 14.601 | 70.312 | 1.00 35.31 |
| ATOM | 5821 | CD1 LEU B 351 | | 63.552 | 14.064 | 68.904 | 1.00 37.88 |
| ATOM | 5822 | CD2 LEU B 351 | | 62.397 | 14.474 | 71.068 | 1.00 39.36 |
| ATOM | 5823 | C LEU B 351 | | 65.662 | 13.065 | 73.240 | 1.00 33.33 |
| ATOM | 5824 | O LEU B 351 | | 64.956 | 12.469 | 74.046 | 1.00 31.48 |
| ATOM | | N LYS B 352 | | 66.915 | 12.720 | 72.981 | 1.00 29.58 |
| ATOM | 5826 | CA LYS B 352 | | 67.527 | 11.576 | 73.633 | 1.00 36.77 |
| ATOM · | | CB LYS B 352 | | 68.457 | 10.864 | 72.647. | 1.00 34.32 |
| ATOM . | | CG LYS B 352 | | 67.777 | 10.563 | 71.326 | 1.00 39.29 |
| ATOM | | CD LYS B 352 CE LYS B 352 | | 68.703 | 9.949 | 70.294 | 1.00 42.25 |
| ATOM | | | | 69.110 | 8.541 | 70.655 | 1.00 46.22 |
| | 2021 | NZ LYS B 352 | | 69.831 | 7.905 | 69.516 | 1.00 44.15 |

Figure 18-89

| | | | | | • | | | |
|------|------|-----|------------------|---|--------|--------------|----------------|------------|
| MOTA | 5832 | С | LYS B 352 | | 68.295 | 11.983 | 74.878 | 1.00 36.30 |
| | | _ | | | | | | |
| ATOM | 5833 | 0 | LYS B 352 | | 69.086 | 12.931 | 74.865 | 1.00 36.65 |
| ATOM | 5834 | N | ASP B 353 | | 68.049 | 11.275 | 75.96 7 | 1.00 30.01 |
| | | | | | | | | |
| MOTA | 5835 | CA | ASP B 353 | | 68.757 | 11.569 | 77.188 | 1.00 33.99 |
| ATOM | 5836 | CB | ASP B 353 | | 67.852 | 11.308 | 78.394 | 1.00 38.57 |
| | | | | | | | | |
| ATOM | 5837 | CG | ASP B 353 | | 67.134 | 9.986 | 78.315 | 1.00 43.90 |
| ATOM | 5838 | OD: | L ASP B 353 | | 66.034 | 9.851 | 78.926 | 1.00 22.39 |
| | | | 2 ASP B 353 | | 67.679 | 9.078 | 77.649 | 1.00 50.42 |
| MOTA | 5839 | | | | | | | |
| ATOM | 5840 | С | ASP B 353 | | 70.022 | 10.723 | 77.202 | 1.00 35.83 |
| ~ | 5841 | 0 | _ASP B 353 | | 70.189 | 9.833 | 76.368 | 1.00 23.71 |
| ATOM | | | | | | | | |
| ATOM | 5842 | N | PRO B 354 | | 70.954 | 11.025 | 78.116 | 1.00 36.36 |
| MOTA | 5843 | CD | PRO B 354 | | 70.928 | 12.093 | 79.132 | 1.00 38.28 |
| • | | | | | | | | |
| ATOM | 5844 | CA | PRO B 354 | - | 72.205 | 10.277 | 78.212 | 1.00 33.62 |
| MOTA | 5845 | CB | PRO B 354 | | 73.003 | 11.104 | 79.213 | 1.00 34.46 |
| | | | PRO B 354 | | | | | |
| MOTA | 5846 | CG | | | 71.896 | 11.556 | 80.164 | 1.00 38.08 |
| ATOM | 5847 | С | PRO B 354 | | 71.924 | 8.883 | 78.733 | 1.00 33.62 |
| | 5848 | · 0 | PRO B 354 | | 70.894 | 8.643 | 79.366 | 1.00 24.82 |
| MOTA | | | | | | | | |
| MOTA | 5849 | И | TRP B 355 | | 72.833 | 7.954 | 78.468 | 1.00 31.76 |
| | 5850 | CA | TRP B 355 | | 72.635 | 6.611 | 78.969 | 1.00 30.01 |
| MOTA | | | | | | | | |
| ATOM | 5851 | CB | TRP B 355 | | 73.653 | 5.655 | 78.359 | 1.00 34.02 |
| MOTA | 5852 | ĊG | TRP B 355 | | 73.025 | 4.378 | 77.910 | 1.00 44.37 |
| | | | | | | | 78.436 | |
| ATOM | 5853 | CD2 | | | 73.263 | 3.072 | | 1.00 45.39 |
| ATOM | 5854 | CE2 | TRP B 355 | | 72.418 | 2.177 | 77.734 | 1.00 44.31 |
| | 5855 | CE3 | | | 74.107 | 2.569 | 79.432 | 1.00 47.19 |
| MOTA | | | | | | | | |
| ATOM | 5856 | CD1 | TRP B 355 | | 72.073 | 4.230 | 76.935 | 1.00 42.18 |
| ATOM | 5857 | NEl | TRP B 355 | | 71.704 | 2.910 | 76.826 | 1.00 37.84 |
| | | | | | | | | |
| ATOM | 5858 | CZ2 | TRP B 355 | | 72.395 | 0.808 | 77.999 | 1.00 44.97 |
| ATOM | 5859 | CZ3 | TRP B 355 | | 74.084 | 1.207 | 79.694 | 1.00 50.83 |
| | 5860 | CH2 | | | 73.231 | 0.341 | 78.979 | 1.00 48.73 |
| ATOM | | | | | | | | |
| MOTA | 5861 | C | TRP B 355 | | 72.819 | 6.685 | 80.485 | 1.00 30.87 |
| | 5862 | 0 | TRP B 355 | • | 73.622 | 7.474 | 80.981 | 1.00 26.93 |
| MOTA | | | | | | | | |
| ATOM | 5863 | N | ARG B 356 | | 72.061 | 5.880 | 81.218 | 1.00 24.96 |
| ATOM | 5864 | CA | ARG B 356 | | 72.147 | 5.848 | 82.671 | 1.00 23.57 |
| | | | | | | 6:319 | 83.257 | 1.00 24.71 |
| MOTA | 5865 | CB | ARG B 356 | | 70.811 | | | |
| MOTA | 5866 | CG | ARG B 356 | | 70.534 | 7.795 | 82.941 | 1.00 23.66 |
| | 5867 | CD | ARG B 356 | | 69.067 | 8.212 | 83.055 | 1.00 20.14 |
| ATOM | | | | | | | | |
| ATOM | 5868 | NE | ARG B 356 | | 68.926 | 9.610 | 82.642 | 1.00 20.59 |
| ATOM | 5869 | CZ | ARG B 356 | | 67.787 | 10.192 | 82.288 | 1.00 25.41 |
| | | | | | | | 82.287 | 1.00 17.01 |
| ATOM | 5870 | NH1 | | | 66.644 | 9.508 | | |
| MOTA | 5871 | NH2 | ARG B 356 | | 67.796 | 11.464 | 81.910 | 1.00 20.07 |
| | 5872 | С | ARG B 356 | | 72.481 | 4.410 | 83.085 | 1.00 26.57 |
| ATOM | | | | | | | | |
| ATOM | 5873 | 0 | ARG B 356 | | 71.610 | 3.641 | 83.485 | 1.00 23.02 |
| ATOM | 5874 | N | GLY B 357 | | 73.761 | 4.063 | 82.978 | 1.00 23.92 |
| | | | | | | | 83.294 | 1.00 25.54 |
| ATOM | 5875 | CA | GLY B 357 | | 74.186 | 2.712 | | |
| ATOM | 5876 | С | GLY B 357 | | 74.796 | 2.464 | 84.657 | 1.00 24.35 |
| ATOM | 5877 | 0 - | GLY B 357 | | 74.523 | 3.161 | 85.628 | 1.00 25.88 |
| | | | | | | | | |
| ATCM | 5878 | N | GLY B 358 | | 75.638 | 1.444 | 84.718 | 1.00 24.32 |
| ATOM | 5879 | CA | GLY B 358 | | 76.282 | 1.070 | 85.960 | 1.00 23.56 |
| | 5880 | C | GLY B 358 | | 76.412 | -0.441 | 85.924 | 1.00 29.26 |
| ATCM | | | | | | | | |
| ATOM | 5881 | 0 | GLY B 358 | | 76.146 | -1.051 | 84.889 | 1.00 23.71 |
| | 5882 | N | GLU B 359 | | 76.814 | ~1.051 | 87.033 | 1.00 27.64 |
| ATOM | | | | | | | | |
| ATOM | 5883 | CA | GLU B 359 | | 76.955 | -2.503 | 87.078 | 1.00 32.16 |
| ATOM | 5884 | CB | GLU B 359 | | 77.822 | -2.936 | 88.265 | 1.00 30.40 |
| | | | | | | | | |
| ATOM | 5885 | CG | GLU B 359 | | 77.125 | -2.772 | 89.601 | 1.00 31.23 |
| ATOM | 5886 | CD | GLU B 359 | | 77.844 | -3.479 | 90.741 | 1.00 37.96 |
| | 5887 | OE1 | GLU B 359 | | 77.287 | -3.521 | 91.861 | 1.00 33.89 |
| ATCM | | | | | | | | |
| ATOM | 5888 | OE2 | GLU B 359 | | 78.959 | -3.990 | 90.520 | 1.00 37.40 |
| ATOM | 5889 | С | GLU B 359 | | 75.571 | -3.122 | 87.261 | 1.00 31.35 |
| | | | | | | -2.429 | 87.588 | 1.00 25.15 |
| ATOM | 5890 | 0 | GLU B 359 | | 74.612 | | | |
| ATOM | 5891 | N | VAL B 360 | | 75.482 | -4.428 | 87.053 | 1.00 29.61 |
| | 5892 | CA | VAL B 360 | | 74.230 | -5.147 | 87.251 | 1.00 26.21 |
| atcm | _ | | | | | - | | |
| ATOM | 5893 | CB | VAL B 360 | | 74.035 | -6.270 | 86.200 | 1.00 28.47 |
| ATOM | 5894 | CG1 | VAL B 360 | | 72.764 | -7.045 | 86.492 | 1.00 22.74 |
| | | | VAL B 360 | | | -5.670 | 84.796 | 1.00 29.70 |
| ATOM | 5895 | _ | | | 73.969 | | | |
| ATOM | 5896 | С | VAL B 360 | | 74.342 | -5.784 | 88.625 | 1.00 26.00 |
| • | 5897 | 0 | VAL B 360 | | 75.150 | -6.693 | 88.821 | 1.00 27.55 |
| ATCM | | | | | | - | | |

Figure 18-90

| | - | | | | | | | |
|--------|--------|-----------|---------|--------|----------|--------|--------|-------|
| ATOM | 5898 | N ARG | B 361 | 73.55 | 3 -5.289 | 89.575 | 1.00 | 26.45 |
| MOTA | 5899 | CA ARG | B 361 | 73.55 | | | | 28.47 |
| ATOM | 5900 | CB ARG | | | | | 1.00 | 28.47 |
| | | | | 72.47 | | 91.787 | 1.00 | 30.55 |
| ATOM | 5901 | CG ARG | | 72.93 | | 92.485 | 1.00 | 32.61 |
| ATOM | 5902 | CD ARG | B 361 | 71.74 | 9 -3.163 | 93.117 | 1.00 | 35.00 |
| ATOM | 5903 | NE ARG | B 361 | 70.85 | | 92.094 | 1 60 | 30.31 |
| ATOM | 5904 | | B 361 | 69.75 | | | 1.00 | 30.31 |
| | 5905 | | | | | 92.350 | 1.00 | 29.45 |
| MOTA | | | B 361 | 69.38 | | 93.605 | | 18.49 |
| ATOM | 5906 | NH2 ARG | B .361 | 69.04 | 1 -1.428 | 91.348 | 1.00 | 30.49 |
| ATOM | 5907 | C ARG | B 361 | 73.35 | | 91.001 | 1 00 | 30.17 |
| ATOM | 5908 | | B 361 | 72.66 | | | 1.00 | 30.17 |
| ATOM | 5909 | N THO | B 362 | | | 90.168 | | 23.60 |
| | | | | 73.949 | | 92.022 | | 33.09 |
| MOTA | 5910 | CA LYS | B 362 | 73.864 | 4 -9.351 | 92.272 | 1.00 | 36.94 |
| ATOM | 5911 | CB LYS | B 362 | 74.68 | | 93.513 | 1 00 | 40.24 |
| MOTA | 5912 | | B 362 | 76.190 | 9.527 | | 1.00 | 40.24 |
| | 5913 | | | | | 93.337 | 1.00 | 52.55 |
| ATOM | | | B 362 | 76.573 | | 92.849 | 1.00 | 56.65 |
| MOTA | 5914 | CE LYS | | 76.149 | 7.032 | 93.819 | 1.00 | 53.39 |
| ATOM | 5915 | NZ LYS | B 362 | 76.553 | | 93.341 | | 48.87 |
| ATOM | 5916 | C LYS | | 72.427 | | 92.463 | | |
| MOTA | 5917 | O LYS | | | | | | 32.84 |
| | | _ | | | -10.867 | 91.938 | | 28.27 |
| ATOM | 5918 | N GLU | | 71.628 | 3 -9.075 | 93.215 | 1.00 | 34.67 |
| ATOM | 5919 | CA GLU | B 363 | 70.245 | -9.493 | 93.435 | 1.00 | 35.72 |
| ATOM | 5920 | CB GLU | B 363 | 69.519 | | 94.390 | 1 00 | 36.04 |
| ATOM | 5921 | | B 363 | | | | | |
| ATOM | | | | 69.502 | | 93.977 | | 44.81 |
| | 5922 | CD GLU | B 363 | 68.859 | | 95.033 | | 52.14 |
| MOTA | 5923 | OE1 GLU | | 67.661 | | 95.341 | 1.00 | 48.46 |
| MOTA | 5924 | OE2 GLU | B 363 | 69.562 | -5.300 | 95.566 | 1 00 | 57.31 |
| ATOM | 5925 | C GLU | | 69.501 | | 92.111 | | |
| ATOM | 5926 | O GLU I | | | | | | 30.68 |
| | | | | 68.695 | | 91.944 | 1.00 | 30.45 |
| MOTA | | N VAL I | | 69.784 | -8.724 | 91.166 | 1.00 | 26.19 |
| MOTA | 5928 | CA VAL I | 3 3 6 4 | 69.138 | -8.789 | 89.852 | 1.00 | 24.65 |
| ATOM | 5929 | CB VAL E | 3 3 6 4 | 69.536 | -7.599 | 88.958 | | 23.49 |
| ATOM | 5930 | CG1 VAL E | | 68.924 | | | | |
| | | CG2 VAL E | | | | 87.563 | 1.00 | 21.01 |
| MOTA | | | | 69.049 | | 89.587 | 1.00 | 23.08 |
| ATOM | - | C VAL E | | 69.530 | -10.083 | 89.144 | 1.00 | 23.19 |
| MOTA | 5933 | O VAL E | 3 364 | 68.691 | -10.749 | 88.542 | | 23.06 |
| ATOM | 5934 | N LYS E | | | -10.436 | 89.216 | | 27.15 |
| ATOM | | CA LYS E | | | | | | |
| | | | | | -11.668 | 88.594 | | 29.18 |
| MOTA | | CB LYS E | | | -11.758 | 88.704 | 1.00 | 28.61 |
| MOTA | 5937 | CG LYS E | | 73.554 | -10.617 | 88.030 | 1.00 | 30.27 |
| ATOM | 5938 | CD LYS B | 365 | | -10.768 | 88.154 | 1.00 | |
| MOTA | 5939 | CE LYS B | 365 | 75.790 | -9.587 | 87.516 | 1.00 | |
| MOTA | | NZ LYS B | | | | | | |
| | | | | 77.271 | -9.689 | 87.606 | 1.00 | |
| MOTA | | C - LYS B | | 70.666 | -12.879 | 89.276 | 1.00 | 25.30 |
| MOTA | 5942 | D LYS B | | 70.282 | -13.837 | 88613 | 1.00 | 26.81 |
| ATOM | 5943 1 | N ASP B | 366 | 70 559 | -12.831 | 90.604 | 1.00 | |
| ATOM | 5944 (| CA ASP B | | 69 963 | -13.938 | 91.347 | 1.00 | 20.10 |
| MOTA | | B ASP B | | 20 205 | 13.330 | | | |
| | | | | | -13.731 | 92.859 | 1.00 | |
| MOTA | | G ASP B | | 71.557 | -13.669 | 93.311 | 1.00 | 32.95 |
| ATOM | 5947 C | D1 ASP B | 366 | 72.446 | -14.099 | 92.551 | 1.00 | 26.37 |
| MOTA | 5948 C | D2 ASP B | 366 | 71.811 | -13.216 | 94.442 | 1.00 | |
| ATOM | 5949 C | | | | -14.110 | 90.986 | | |
| | | | | | | | 1.00 | |
| MOTA | 5950 C | | | | -15.231 | 90.869 | 1.00 2 | |
| ATOM | 5951 N | THR B | 367 | 67.777 | -13.002 | 90.801 | 1.00 2 | 28.63 |
| ATOM | 5952 C | A THR B | 367 | | -13.080 | 90.438 | 1.00 2 | |
| ATOM | | B THR B | | | -11.683 | 90.359 | 1.00 | |
| MOTA | | G1 THR B | | | | | | |
| | | | | | -11.068 | 91.656 | 1.00 2 | 28.12 |
| MOTA | | | 367 | 64.280 | -11.786 | 89.890 | 1.00 2 | 22.94 |
| MOTA | 5956 C | THR B | 367 | 66.197 | -13.782 | 89.094 | 1.00 2 | 25.46 |
| ATOM | 5957 O | | 367 | | -14.693 | 88.964 | 1.00 2 | 4 40 |
| ATOM | 5958 N | | 368 | | | | 1 00 2 | 77.40 |
| | | | | | -13.361 | 88.092 | 1.00 2 | |
| ATOM | 5959 C | | | | -13.990 | 86.785 | 1.00 2 | 8.99 |
| ATOM | 5960 C | B LEU B | 368 | 67.719 | -13.256 | 85.759 | 1.00 2 | 7.67 |
| ATOM · | 5961 C | G LEU B | 368 | 67.060 | | 85.046 | 1.00 2 | 9 47 |
| ATOM | | D1 LEU B | | 65.923 | -12 607 | 84.195 | 1.00 3 | 2 45 |
| | | D2 LEU B | | | | | 1 00 - | 2.43 |
| HOTA | 5963 C | U4 | -00 | 66.546 | -11.027 | 86.043 | 1.00 1 | 9.43 |

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| | | | | | | | | | | • | | |
|------------------|----------------------|----------|------------|-----|--------------|---|------------------|-----|--------------------|--------------------|------|----------------|
| ATOM | 5964 | С | LE | ; в | 368 | | 67.26 | 2 | -15.454 | 86.888 | 1.00 | 32.40 |
| ATOM | 5965 | 0 | LE | : в | 368 | | 66.72 | 6 | -16.309 | 86.179 | 1.00 | 31.80 |
| ATOM | 5966 | N | | | 369 | | 68.21 | .2 | -15.735 | 87.774 | 1.00 | 33.59 |
| MOTA | 5967 | CA | | | 369 | | | | -17.101 | 88.003 | | 39.68 |
| MOTA | 5968 | | | | 369 | | | | -17.141 | 89.082 | | 42.61 |
| ATOM | 5969 | CG | | | 369 | | | | -17.138 | 88.537 | | 50.65 |
| ATOM | 5970 | CD | | | 369 | | | | -18.443 | 87.842 | | 55.81 |
| MOTA | 5971 | OE. | | | 369 | | | | -18.561 | | | 57.42 |
| MOTA | 5972 | OE: | | | 369 | | | | -19.353 | 87.841 | | 58.37 |
| ATOM | 5973 | C | | | 369 | | | | -17.954 | 88.442 | | 34.94 |
| MOTA | 5974 | 0 | | | 369 | | | | -18.974 | 87.827 | | 32.71 |
| ATOM | 5975 | N | | | 370 | | | | -17.541 | 89.512 | | 34.92 |
| ATOM | 5976 | CA | | | 370 | | | | -18.295 | 89.993 | | 35.12 |
| ATOM | 5977 | CB | | | 370 370 | | | | -17.679 -17.916 | 91.268 | | 37.39 |
| MOTA | 5978 5979 | CD | | | 370 | | | | -17.910 -16.741 | 92.532 92.892 | | 44.70 48.10 |
| MOTA | 5980 | CE | | | 370 | | | | -15.537 | 93.346 | _ | 47.82 |
| MOTA | 5981 | NZ | | | 370 | | | | -14.387 | 93.786 | | 45.41 |
| MOTA MOTA | 5982 | C | | | 370 | - | | | -18.375 | 88.930 | | 33.21 |
| MOTA | 5983 | ō | | | 370 | | | | -19.409 | 88.773 | | 29.52 |
| ATOM | 5984 | N | | | 371 | | | | -17.288 | 88.191 | | 31.62 |
| ATOM | 5985 | CA | | | 371 | | 63.36 | | -17.274 | 87.153 | | 37.19 |
| ATOM | 5986 | CB | | | 371 | | | | -15.938 | 86.403 | | 35.65 |
| ATOM | 5987 | С | ALA | В | 371 | • | | | -18.431 | 86.181 | | 37.79 |
| ATOM | 5988 | 0 | ALA | В | 371 | | 62.62 | 7 | -19.137 | 85.838 | 1.00 | 34.45 |
| ATOM | 5989 | N | LYS | В | 372 | | 64.81 | 0 | -18.644 | 85.759 | 1.00 | 40.10 |
| ATOM | 5990 | CA | LYS | В | 372 | | 65.14 | 7 | -19.698 | 84.792 | 1.00 | 40.46 |
| ATOM | 5991 | C | | | 372 | | | | -21.066 | 85.348 | | 43.15 |
| ATOM | 5992 | 0 | LYS | | 372 | | | | -22.053 | 84.591 | | 43.57 |
| MOTA | 5993 | CB | | | 372 | | | | -19.694 | 84.517 | | 40.51 |
| ATOM | 5994 | CG | LYS | | 372 | | | | -18.925 | 83.248 | | 20.00 |
| ATOM | 5995 | CD | | | 372 | • | 68.35 | | -19.390 | 82.635 | | 20.00 |
| ATOM | 5996 | CE | | | 372 372 . | | | | -20.907 | 82.706 | | 20.00 |
| ATOM | 599 7 5998 | NZ N | LYS ALA | | 373 | | | | -21:354 -21:159 | 82.116 86.624 | | 47.80 |
| ATOM | 5999 | CA | ALA | | 373 | | | | -22.425 | 87.239 | | 49.71 |
| ATOM ATOM | 6000 | CB | ALA | | | | 64.76 | | -22.639 | 88.546 | | 48.25 |
| ATOM | 6001 | c | ALA | | 373 | | 62.51 | | -22.443 | 87.494 | | 53.38 |
| MOTA | 6002 | ŏ | ALA | | 373 | | 61.84 | | -23.313 | | | 58.01 |
| ATOM | 6003 | OXT | | | | | | | -21.589 | 88.269 | 1.00 | 55.13 |
| HETATM | | ZN | ZN | С | 1 | | 49.66 | | 9.211 | 109.302 | 1.00 | 32.54 |
| HETATM | | 01 | TSA | D | 2 | | 47.66 | 9 | 8.189 | 109.464 | 1.00 | 28.76 |
| HETATM | | G2 | TSA | | 2 | | 49.95 | | 6.981 | 108.340 | | 25.81 |
| HETATM | | 03 | TSA | | 2 | | 52.45 | | 5.101 | 101.667 | | 36.93 |
| HETATM | 2995 | N1 | TSA | | 2. | | 47.80 | | 7.789 | 108.131 | | 31.21 |
| HETATM | | N2 | TSA | | 2 ' | | 53.01 | | -1.329 | 101.259 | | 30.57 |
| HETATM | | C1 | TSA | | 2 | | 51.85 | | 2.799 | 101.610 | | 28.47 |
| HETATM | 2998 | C2 | TSA | | 2 | | 50.90 | | 1.769 | 101.666 | | 25.57 |
| HETATM | 2999 | C3 | TSA TSA | | 2 | | 51.243 | | | 101:551 | | 21.68 |
| HETATM | 3000 | C4 | | _ | 2 2 | | 52.626 53.589 | D . | | 101.366 | | 25.02 |
| HETATM HETATM | 3003 | C5 C6 | TSA TSA | | 2 | | 53.21 | | | 101.303 101.418 | | 29.24 |
| HETATM | 3002 | C7 | TSA | | 2 | | 51.57 | | | 101.734 | | 32.98 |
| HETATM | 3003 | C8 | TSA | | 2 | | 50.108 | | | 101.996 | | 29.05 |
| HETATM | 3005 | C9 | TSA | | 2 | | 50.052 | | | 103.338 | _ | 28.13 |
| HETATM | 3006 | | TSA | | 2 | | 49.060 | | | 104.279 | | 25.99 |
| HETATM | 3007 | | TSA | | 2 | | 49.315 | | | 105.504 | | 32.05 |
| HETATM | 3008 | | TSA | | 2 | | 48.515 | | | 106.595 | | 27.37 |
| HETATM | 3009 | | TSA | | 2 | | 48.85 | | | 107.756 | | 29.02 |
| HETATM | 3010 | | TSA | | 2 | | 49.680 | | | 100.864 | | 30.21 |
| HETATM | 3011 | | TSA | | 2 | | 47.776 | | | 104.132 | 1.00 | 30.60 |
| HETATM | 3012 | | TSA | | 2 | | 54.438 | | -1.703 | 101.139 | | 23.45 |
| HETATM | 3013 | | TSA | | 2 | | 52.044 | 1 | | 101.316 | | 23.15 |
| HETATM | 6004 | ZN | | E | 1 | | 52.949 | | 1.842 | 85.681 | | 28.19 |
| HETATM | 6005 | 01 | TSA | | 2 | | 50.964 | | 0.911 | 85.428 | | 24.72 |
| HETATM | 6006 | 02 | TSA | F | 2 | | 51.255 | 5 | 3.324 | 86.654 | 1.00 | 30.24 |

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| HETATM 6007 O3 TSA F 2 | |
|---|---|
| | 51.569 6.512 93.219 1.00 27.89 |
| HETATM 6008 N1 TSA F 2 | |
| HETATM 6009 N2 TSA F 2 | 45 45 47.43 |
| HETATM 6010 C1 TSA F 2 | 10 10.24 |
| *************************************** | 49.443 7.579 93.304 1.00 27 18 |
| | 48.035 7.529 93.267 1.00 25.98 |
| HETATM 6012 C3 TSA F 2 | 33.207 1.00 25.98 |
| HETATM 6013 C4 TSA F 2 | 45 45 45 45 45 45 45 45 45 45 45 45 45 4 |
| | 47.837 9.971 93.583 1.00 25.75 |
| | 49.274 10.017 93.626 1.00 26.53 |
| HETATM 6015 C6 TSA F 2 | |
| HETATM 6016 C7 TSA F 2 | 50 2.00 28.30 |
| | 1.00 23.27 |
| Types my coac | · 49./16 5.006 92.905 1 nn 24 19 |
| | |
| HETATM 6019 C10 TSA F 2 | 10 27.20 |
| HETATM 6020 C11 TSA F 2 | 100 30.21 |
| T10000 1 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | 50.118 3.553 89.327 1.00 27.18 |
| | 49.762 2.624 88.409 1.00 23.47 |
| HETATM 6022 C13 TSA F 2 | |
| HETATM 6023 C14 TSA F 2 | 50 100 20.20 |
| | 50.208 4.019 93.994 1.00 28.83 |
| | 40.013 3.270 90.863 1.00 26 16 |
| HETATM 6025 C17 TSA F 2 | |
| HETATM 6026 C16 TSA F 2 | 42 222 |
| HETATM 6027 OH2 WAT G 1 | |
| | 61.391 6.723 88.062 1.00 12.93 |
| Troms on a cons | 55.595 -4.443 83.558 1.00 7.53 |
| HETATM 6029 OH2 WAT G 3 | |
| HETATM 6030 OH2 WAT G 4 | 1.00 12.33 |
| HETATM 6031 OH2 WAT G 5 | 45 505 45 45 45 45 45 45 45 45 45 45 45 45 45 |
| Transme Cons | 45.523 13.627 76.224 1.00 11.14 |
| HETATM 6032 OH2 WAT G 6 | 24.466 -6.064 85.688 1.00 22.41 |
| HETATM 6033 OH2 WAT G 7 | |
| HETATM 6034 OH2 WAT G 8 | |
| HETATM 6035 OH2 WAT G 9 | |
| HETATM 6036 OH2 WAT G 10 | 48.554 -14.901 83.717 1.00 23 94 |
| | 57.540 -7.620 122.771 1.00 26.96 |
| HETATM 6037 OH2 WAT G 11 | |
| HETATM 6038 OH2 WAT G 12 | 04.025 1.00 22.51 |
| HETATM 6039 OH2 WAT G 13 | |
| HETATM 6040 OH2 WAT G 14 | 62.335 10.679.117.140 1.00 19.47 |
| Imma ma coas | 45.565 9:469 79.366 1.00 18.81 |
| HETATM 6041 OH2 WAT G 15 | 43.311 8.237 79.508 1.00 26.11 |
| HETATM 6042 OH2 WAT G 16 | 20.11 |
| HETATM 6043 OH2 WAT G 17 | |
| | 40.672 2.507 81.576 1.00 18.30 |
| HETATM 6044 OH2 WAT G 18 | 61.830 10.923 77.709 1.00 22.27 |
| HETATM 6045 OH2 WAT G 19 | |
| HETATM 6046 OH2 WAT G 20 | |
| HETATM 6047 OH2 WAT G 21 | 2.00 30.00 |
| ************************************** | 36.382 -8.352 88.841 1.00 17.32 |
| HETATM 6048 OH2 WAT G 22 | 39.316 -10.091 86.422 1.00 27.38 |
| HETATM 6049 OH2 WAT G 23 | 54.802 -3.446 90.346 1.00 21.73 |
| HETATM 6050 OH2 WAT G 24 | 1.00 21,73 |
| HETATM 6051 OH2 WAT G 25 | |
| TTPM3 MM COEO DIA | 56.747 8.830 60.744 1.00 40.67 |
| HETATM 6052 OH2 WAT G 26 | 41.952 9.79 100.118 1.00 27 92 |
| HETATM 6053 OH2 WAT G 27 | 31.268 2.80; 106.695 1.00 24.31 |
| HETATM 6054 OH2 WAT G 28 | |
| HETATM 6055 OH2 WAT G 29 | 1.00 30.93 |
| TIMES CALC. | |
| 11000 COET 0100 | 39.287 9.257 85.623 1 00 22 64 |
| HETATM 6057 OH2 WAT G 31 | 61.221 14.462 87.256 1.00 29.85 |
| HETATM 6058 OH2 WAT G 32 | |
| HETATM 6059 OH2 WAT G 33 | |
| HETATM 6060 CH2 WAT G 34 | 64.657 -2.682 96.225 1.00 18.70 |
| | 44.059 -2.698 99.805 1.00 30.02 |
| HETATM 6061 OH2 WAT G 35 | 38.480 4.763 93.051 1.00 28.03 |
| HETATM 6062 OH2 WAT G 36 | 1.00 20.03 |
| tromators (DC) otto | |
| | 57.092 3.145 93.309 1.00 22.31 |
| | 52.194 -1.400 118.878 1.00 30.83 |
| HETATM 6065 OH2 WAT G 39 | 69.400 14.200 123.379 1.00 30.98 |
| HETATM 6066 OH2 WAT G 40 | 24 024 |
| HETATM 6067 CH2 WAT G 41 | 15.00 30.13 |
| HETATM 6068 OH2 WAT G 42 | 46.657 -10.880 89.402 1.00 29.24 |
| | 24.976 13.489 109.692 1.00 46.34 |
| HETATM 6069 OH2 WAT G 43 | 46.533 -4.511 94.759 1.00 23.11 |
| HETATM 6070 OH2 WAT G 44 | 51 440 45.11 |
| HETATM 5071 OH2 WAT G 45 | 70 700 |
| HETATM 6072 OH2 WAT G 46 | 70.578 4.183 105.248 1.00 42.42 |
| HETATM 6072 OH2 WAT G 46 | 53.938 -9.936 116.021 1.00 38.97 |
| | |

```
-0.443 63.035
                                                           1.00 28.35
                          47
                                  38.458
HETATM 6073
              OH2 WAT G
                                                           1.00 34.46
                                          7.930 107.466
              OH2 WAT G
                                  64.786
                          48
HETATM 6074
                                                           1.00 40.51
                                          36.521 114.809
                                  50.823
              OH2 WAT G
                          49
HETATM 6075
                                                           1.00 39.11
                                                   68.080
              OH2 WAT G
                          50
                                  33.963 -10.352
HETATM 6076
                                                           1.00 33.30
                                  71.328 -14.321
                                                   86.007
                          51
              OH2 WAT G
HETATM 6077
                                  63.272 10.210
                                                   79.836
                                                           1.00 35.75
              OH2 WAT G.
                          52
HETATM 6078
                                                           1.00 29.57
                                                   94.306
                          53
                                  59.263 -12.096
              OH2 WAT G
RETATM 6079
                                                   76.561
                                                           1.00 27.97
                                  46.041 10.641
              OH2 WAT G
                          54
HETATM 6080
                                  46.614 -13.620
                                                   89.775
                                                           1.00 24.25
                          55
              OH2 WAT G
HETATM 6081
                                                           1.00 29.19
                                  76.600
                                           0.622
                                                   89.097
                          56
              OH2_WAT G
HETATM 6082
                                                           1.00 34.05
                                                   79.089
                                           6.439
                                  53.555
HETATM 6083
              OH2 WAT G
                          57
                                                   83.310
                                                           1.00 35.02
                                          11.026
              OH2 WAT G
                          58
                                  71.301
HETATM 6084
                                                   81.594
                                          -9.956
                                                           1.00 33.21
                                  28.188
              OH2 WAT G
                         59
HETATM 6085
                                                           1.00 27.64
                                          20.992
                                                   98.483
HETATM 6086
              OH2 WAT G
                          60
                                  53.084
                                                           1.00 30.30
                                                   93.423
                                  59.484
                                           8.630
              OH2 WAT G
                          61
HETATM 6087
                                  26.195
                                          -3.809
                                                   95.805
                                                           1.00 33.04
              OH2 WAT G
                          62
HETATM 5088
                                                           1.00 37.39
                                                   89.620
              OH2 WAT G
                          63
                                  26.095
                                          -0.121
HETATM 6089
                                          -6.141 109.711
                                                           1.00 20.88
                                  47.100
              OH2 WAT G
                          64
HETATM 6090
                                  23.273
                                           0.731
                                                   92.275
                                                           1.00 30.38
              OH2 WAT G
                          65
HETATM 6091
                                                            1.00 37.51
                                  45.340 -24.751
                                                   72.694
HETATM 6092
              OH2 WAT G
                          66
                                  33.754
                                          16.234 111.676
                                                            1.00 34.63
                          67
              OH2 WAT G
HETATM 6093
                                                           1.00 47.11
                                                 126.276
                                          19.209
              OH2 WAT G
                          68
                                  52.831
HETATM 6094
                                          16.953 111.099
                                                            1.00 26.24
                                  50.218
HETATM 6095
              OH2 WAT G
                          69
                                           5.844
                                                   70.857
                                                            1.00 24.95
                          70
                                  44.791
              OH2 WAT G
HETATM 6096
                                                            1.00 29.48
                                  49.517 -18.731
                                                   82.921
              OH2 WAT G
                          71
HETATM 6097
                                          10.131 116.550
                                                            1.00 48.70
                                  76.379
                          72
              OH2 WAT G
HETATM 6098
                                                            1.00 46.35
                                          -8.086
                                  30.214
                                                   87.873
                          73
HETATM 6099
              OH2 WAT G
                                                            1.00 30.80
                                                   80.458
                          74
                                  45.320
                                          12.061
              OH2 WAT G
HETATM 6100
                                                            1.00 29.04
                                            5.360
                                                   86.249
              OH2 WAT G
                          75
                                  72.881
HETATM 6101
                                                   87.252
                                                            1.00 41.96
                                  59.674 -23.046
                          76
HETATM 6102
              OH2 WAT G
                                                            1.00 26.45
                                            7.921
                                                  100.345
                          77
                                  40.619
              OH2 WAT G
HETATM 6103
                                                            1.00 36.27
                                                   70.073
                                  41.666 -19.477
              OH2 WAT G
                          78
HETATM 6104
                                  46.408
                                                   92.717
                                                            1.00 25.78
                                          -6.539
                          79
HETATM 6105
              OH2 WAT G
                                                   81.646
                                                            1.00 28.34
                                  35.743 -12:230
              OH2 WAT G
                          80
HETATM 6106
                                                            1.00 41.15
                                            8.745 121.961
              OH2 WAT G
                                  28.268
                          81
HETATM 6107
                                  68.843
                                            3.154
                                                   71.986
                                                            1.00 32.34
                          82
              OH2 WAT G
HETATM 6108
                                  52.125 -11.158
                                                   85.150
                                                            1.00 24.14
              OH2 WAT G
HETATM 6109
                          83
                                                   92.264
                                                            1.00 26.12
                                  75.374
                                          -1.773
              OH2 WAT G
                          84
HETATM 6110
                                                            1.00 37.07
                                          12.230
                                                  142.271
                          85
                                  46.957
              OH2 WAT G
HETATM 6111
                                  63.789
                                            9.551
                                                   64.329
                                                            1.00 55.58
HETATM 6112
              OH2 WAT G
                          86
                                                            1.00 58.55
                                          21.185
                                                   72.215
                          87
                                  60.672
              OH2 WAT G
HETATM 6113
                                                            1.00 31.10
                                                   82.064
                          88
                                  56.547
                                            9.505
HETATM 6114
              OH2 WAT G
                                                   92.250
                                  26.366
                                          -0.876
                                                            1.00 29.70
                          89
              OH2 WAT G
 HETATM 6115
                                                   80.808
                                                            1.00 32.85
                                  67.604 -16.583
              OH2 WAT G
                          90
HETATM 6116
                                            1.899
                                                   82.068
                                                            1.00 42.95
              OH2 WAT G
                          91
                                  23.910
HETATM 6117
                                                            1.00 30.05
                                                  117.380
                                  50.032
                                            4.106
                          92
              OH2 WAT G
 HET/ TM 6118
                                  26.774
                                                   83.952
                                                            1.00 43.59
                                          -9.492
              OH2 WAT G
HET. IM 6119
                          93
                                                  113.787
                                                            1.00 40.17
                                           -0.637
              OH2 WAT G
                          94
                                  42.714
 HETA.M 6120
                                                            1.00 47.82
                                  57.966
                                            7.989 134.170
                         95
 HETATM 6121
              OH2 WAT G
                                           -3.550 119.086
                                                            1.00 36.62
                                  54.478
HETATM 6122
              OH2 WAT G
                          96
                                          11.696 101.718
                                                            1.00 41.62
                         97
                                  53.065
              OH2 WAT G
HETATM 6123
                                                            1.00 45.98
                                          -23.645
                                                   68.207
                                  58.286
                         98
 HETATM 6124
              OH2 WAT G
                                          -9.614 121.975
                                                            1.00 34.57
                                  54.855
              OH2 WAT G
                        99
HETATM 6125
                                                   57.145
                                                            1.00 42.14
                                  57.408
                                           -3.352
              OH2 WAT G 100
 HETATM 6126
                                          20.353 123.667
                                                            1.00 33.87
                                  63.590
              OH2 WAT G 101
 HETATM 6127
                                  48.129 -23.143
                                                   72.392
                                                            1.00 30.23
              OH2 WAT G 102
 HETATM 6128
                                                   76.094
                                                            1.00 52.01
                                  62.834
                                            6.913
              OH2 WAT G 103
HETATM 6129
                                                   73.089
                                                            1.00 36.29
                                  34.566
                                            6.529
              OH2 WAT G 104
 HETATM 6130
                                                   67.459
                                                            1.00 36.85
                                  51.588
                                           20.869
              OH2 WAT G 105
 HETATM 6131
                                                            1.00 42.87
                                                  129.379
                                  28.160
                                           18.020
              OH2 WAT G 106
HETATM 6132
                                                            1.00 43.62
                                                   57.603
                                  49.082 -11.452
              OH2 WAT G 107
 HETATM 6133
                                                            1.00 41.95
                                                   93.281
                                          -8,605
                                  44.717
              OH2 WAT G 108
 HETATM 6134
                                                            1.00 35.71
                                                   94.019
                                  67.088
                                          -11.900
              OH2 WAT G 109
HETATM 6135
                                                            1.00 35.40
                                          22.763 100.800
                                  49.561
              OH2 WAT G 110
 HETATM 6136
                                                            1.00 56.20
                                           10.960 124.536
                                  75.853
              OH2 WAT G 111
 HETATM 6137
                                            8.930 136.095 1.00 36.40
              OH2 WAT G 112
                                   54.383
HETATM 6138
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HETATM 6139
                 OH2 WAT G 113
                                     33.114
                                              1.764
                                                     67.443
                                                              1.00 37.01
  HETATM 6140
                OH2 WAT G 114
                                     42.618
                                             -4.357 102.345
                                                              1.00 39.18
  HETATM 6141
                 OH2 WAT G 115
                                     53.605
                                            -10.816
                                                      66.281
                                                              1.00 31.62
  HETATM 6142
                OH2 WAT G 116
                                     73.410
                                             -1.010
                                                      90.400
                                                              1.00
                                                                   34.72
  HETATM 6143
                OH2 WAT G 117
                                    68.899
                                              3.789 110.221
                                                              1.00 35.69
  HETATM 6144
                OH2 WAT G 118
                                             19.159 112.425
                                    31.474
                                                              1.00 28.08
  HETATM 6145
                OH2 WAT G 119
                                    39.749
                                             -0.616 132.457
                                                              1.00 37.43
                OH2 WAT G 120
  HETATM 6146
                                    44.921
                                              1.089 137.137
                                                              1.00 40.80
  HETATM 6147
                OH2 WAT G 121
                                    31.081
                                                     75.105
                                              7.617
                                                              1.00 40.86
  HETATM 6148
                OH2 WAT G 122
                                    35.554
                                             12.017 105.965
                                                              1.00 33.58
  HETATM 6149
                OH2
                    WAT G 123
                                    41.381
                                            -23.534
                                                     70.872
                                                              1.00 38.10
  HETATM 6150
                OH2 WAT G 124
                                    31.999
                                              1.992
                                                     73.813
                                                              1.00 33.97
  HETATM 6151
                                    55.761
                OH2 WAT G 125
                                             10.285 101.654
                                                              1.00 47.66
  HETATM 6152
                OH2
                    WAT G 126
                                             12.964 133.642
                                    30.596
                                                              1.00 37.98
  HETATM 6153
                OH2 WAT G 127
                                    59.611
                                             5.347,136.114
                                                              1.00 46.39
  HETATM 6154
                OH2 WAT G 128
                                    24.190
                                             12.220 124.679
                                                              1.00 30.77
  HETATM 6155
                OH2
                    WAT G 129
                                    70.078
                                             4.455
                                                    86.283
                                                              1.00 36.11
  HETATM 6156
                   WAT G 130
                OH2
                                            -4.314 125.597
                                    57.882
                                                              1.00 41.40
  HETATM 6157
                OH2 WAT G 131
                                    45.838 -20.690
                                                              1.00 35.98
                                                     65.884
  HETATM 6158
                    WAT G 132
                OH2
                                    47.574
                                             3.186
                                                     79.027
                                                              1.00 36.67
  HETATM 6159
                   WAT G
                OH2
                          133
                                    46.856
                                           -18.901
                                                     62.295
                                                             1.00 45.40
  HETATM 6160
                OH2 WAT G 134
                                    40.164
                                             5.047
                                                     95.358
                                                             1.00 31.38
 HETATM 6161
                OH2 WAT G 135
                                    27.268
                                            -0.405 122.461
                                                             1.00 38.16
               OH2 WAT G 136
 HETATM 6162
                                    54.200
                                           -20.155
                                                     66.212
                                                             1.00 37.55
 HETATM 6163
               OH2 WAT G 137
                                    45.435
                                           ~10.534 103.626
                                                             1.00 37.96
 HETATM 6164
               OH2 WAT G 138
                                    31.633
                                            25.030 106.499
                                                             1.00 43.94
 HETATM 6165
               OH2 WAT G 139
                                    79.029
                                            -7.518
                                                     93.606
                                                             1.00 40.55
 HETATM 6166
               OH2 WAT G 140
                                   68.597
                                            20.711 111.685
                                                             1.00
                                                                  33.25
 HETATM 6167
               OH2 WAT G
                         141
                                   64.263
                                             8.524 113.832
                                                             1.00 40.63
 HETATM 6168
               OH2 WAT G 143
                                   49.387
                                           -24.485
                                                    70.152
                                                             1.00 34.07
 HETATM 6169
               OH2
                   WAT G 144
                                   23.383
                                            -3.854
                                                     83.604
                                                             1.00 32.22
 HETATM 6170
               OH2 WAT G 145
                                   42.360
                                            -0.710
                                                     61.686
                                                             1.00 35.94
               OH2 WAT G 146
 HETATM 6171
                                   34.421
                                            -3.304
                                                     65.685
                                                             1.00 35.42
 HETATM 6172
               OH2
                   WAT G 147
                                   31.506
                                             3.409
                                                    89.579
                                                             1.00 39.86
               OH2 WAT G 148
 HETATM 6173
                                            10.688
                                   34.963
                                                    91.806
                                                             1.00 31.12
 HETATM 6174
               OH2 WAT G 149
                                   54.859
                                           -15.085
                                                    96.769
                                                             1.00 46.65
 HETATM 6175
               OH2 WAT G 150
                                   34.695
                                             2.391
                                                   131.273
                                                             1.00 39.22
 HETATM 6176
               OH2 WAT G 151
                                   40.348
                                                    61.905
                                             1.395
                                                             1.00 34.09
 HETATM 6177
               OH2 WAT G 152
                                   66.912
                                           17.666
                                                   127.489
                                                             1.00 45.19
 HETATM 6178
               OH2 WAT G 153
                                   31.096
                                                   103.232
                                           19.900
                                                             1.00 43.45
 HETATM 6179
               OH2
                  WAT G 154
                                   28.074
                                           -4.222
                                                    70.175
                                                             1.00 28.86
 HETATM 6180
              он2
                  WAT G 155
                                   63.586
                                           -1.894
                                                    99.003
                                                             1.00 41.15
 HETATM 6181
              OH2
                  WAT G 156
                                   54.145
                                          -22.222
                                                    88.415
                                                             1.00 40.92
              OH2 WAT G 157
 HETATM 6182
                                   62.443
                                           13.765
                                                    89.547
                                                             1.00 33.69
 HETATM 6183
                  WAT G 158
              OH2
                                   58.832
                                            9.798
                                                   101.311
                                                             1.00 31.00
 HETATM 6184
              OH2 WAT G 159
                                   37.701
                                           -5.528
                                                   119.322
                                                             1 00 45.00
HETATM 6185
                  WAT G 160
              OH2
                                   43.599
                                           13.442
                                                   131.274
                                                             1 00 38.43
HETATM 6186
              OH2
                  WAT G 161
                                  23.540
                                           -1.137
                                                    96.111
                                                            1 00 51.83
HETATM 6187
              OH2
                  WAT G 162
                                  59.915
                                           -4.318
                                                  110.873
                                                            1.00 41.92
HETATM 6188
              OH2 WAT G 163
                                  51.265
                                           -8.264
                                                    60.546
                                                            1.00 31.25
HETATM 6189
              OH2
                  WAT G 164
                                  58.109
                                            7.024
                                                    98.294
                                                            1.00 46.30
HETATM 6190
              OH2 WAT G 165
                                  46.553
                                           18.195
                                                    74.179
                                                            1.00 37.53
HETATM 6191
              OH2 WAT G 166
                                  55.706
                                                            1.00 43.91
                                          -21.025
                                                    92.515
HETATM 6192
              OH2
                  WAT G 167
                                  67.146
                                           -1.958
                                                  109.704
                                                            1.00 43.13
HETATM 6193
              OH2 WAT G 168
                                  47.445
                                           -3.047 134.746
                                                            1.00 27.99
HETATM 6194
              OH2 WAT G 169
                                  65.193
                                            5.304
                                                   63.562
                                                            1.00 36.05
HETATM 6195
             OH2
                 WAT G 170
                                                  102.024
                                  36.176
                                            8.979
                                                            1.00 39.63
HETATM 6196
             OH2 WAT G 171
                                  70.527
                                            5.797
                                                   70.886
                                                            1.00 44.69
HETATM 6197
             OH2 WAT G 172
                                  67.166
                                            8.735
                                                   74.628
                                                            1.00 51.41
HETATM 6198
             OH2 WAT G 173
                                  19.700
                                            9.630
                                                   81.850
                                                            1.00 53.49
HETATM 6199
             OH2 WAT G 174
                                  55.875
                                          11.277
                                                   87.176
                                                            1.00 38.63
HETATM 6200
             OH2 WAT G 175
                                  61.874
                                            8.432
                                                   91.682
                                                            1.00 40.08
HETATM 6201
             OH2 WAT
                     G 176
                                  36.771
                                          -6.815
                                                  121.530
                                                            1.00 32.57
HETATM 6202
             OH2 WAT G 177
                                  63.224
                                           7.776
                                                   89.317
                                                            1.00 29.83
HETATM 6203
             OH2 WAT G 178
                                 29.606
                                          15.345
                                                  132.470
                                                            1.00 47.28
HETATM 6204
             OH2 WAT G 179
                                  52.811
                                          11.799
                                                  98.957
                                                            1.00 36.09
```

| HETATM | 6205 | OH2 | WAT G | 180 | 38.58 | 18.249 | 88.356 | 1.00 36.19 |
|--|--|--|---|---|---|--|---|--|
| HETATM | 6206 | OH2 | WAT G | | 43.73 | 4 -15.681 | 61.135 | 1.00 34.24 |
| HETAIM | 8200 | | | | | | 91.437 | 1.00 37.96 |
| HETATM | 6207 | OH2 | | | 42.28 | 3 15.251 | | • |
| HETATM | 6208 | OH2 | WAT G | 183 | 57.12 | 1 -11.129 | 126.206 | 1.00 45.78 |
| HEIRIH | 6200 | OH2 | | | | 1 -19.367 | 92.127 | 1.00 36.55 |
| HETATM | 6209 | | | | | | .95.969 | 1.00 39.12 |
| HETATM | 6210 | OH2 | WAT G | 185 | 56.88 | 2.453 | | |
| HETATM | 6211 | OH2 | WAT G | 186 | 26.35 | 6 14.125 | 125.052 | 1.00 32.68 |
| MEINIM | 6010 | | | | 24.63 | 1 20 230 | 122.650 | 1.00 45.67 |
| HETATM | 6212 | | WAT G | | | | | |
| HETATM | 6213 | OH2 | WAT G | .188 | 23.51 | 6 4.964 | 81.599 | 1.00 42.16 |
| HETATM | 6211 | OH2 | WAT G | 189 | 55.01 | 7 14.964 | 62.948 | 1.00 50.18 |
| HEIAIN | 0214 | | | | 33.37 | | 105.640 | 1.00 37.04 |
| HETATM | 6215 | | WAT G | | | | | |
| HETATM | 6216 | OH2 | WAT G | 191 | ,44.46 | 6 -10.386 | 91.144 | 1.00 36.62 |
| HETATM | 6217 | | WAT G | | 28.43 | 7 22.668 | 121.285 | 1.00 38.19 |
| HEIAIM | 0217 | | | | 29.78 | | 122.112 | 1.00 42.05 |
| HETATM | 6218 | OH2 | WAT G | | | | | |
| HETATM | 6219 | OH2 | WAT G | | 28.85 | | 96.101 | 1.00 48.35 |
| HETATM | 6220 | OH2 | WAT G | 195 | 41.68 | 1 11.318 | 92.011 | 1.00 32.60 |
| | | | WAT G | 106 | 26 91 | 2 -10.229 | 111 631 | 1.00 47.70 |
| HETATM | 6221 | OH2 | | | . 20.01 | | | 1.00 48.86 |
| HETATM | 6222 | OH2 | WAT G | 197 | | 2 -23.250 | 76.629 | |
| HETATM | 6223 | OH2 | WAT G | 198 | 25.48 | 4 12.756 | 121.410 | 1.00 43.09 |
| ULIAIM | CD 2 4 | | | | | 4 -20.514 | 111 706 | 1.00 46.80 |
| HETATM | 5224 | OH2 | WAT G | | | | | 1.00 44.89 |
| HETATM | 6225 | OH2 | WAT G | 200 | | 3 -13.079 | 95.699 | |
| HETATM | 6226 | OH2 | WAT G | 201 | 59.98 | 2 24.381 | 103.984 | 1.00 40.63 |
| | | | WAT G | | | 412.771 | 74.705 | 1.00 35.13 |
| HETATM | | | | | | | | 1.00 33.53 |
| HETATM | 6228 | OH2 | WAT G | | 28.70 | | 79.238 | |
| HETATM | | OH2 | WAT G | 204 | 53.25 | 6 -3.576 | 122.243 | 1.00 48.49 |
| MEININ | 6220 | | WAT G | | 50.70 | | 87.357 | 1.00 41.26 |
| HETATM | 6230 | | | | | | | 1.00 39.15 |
| HETATM | 6231 | OH2 | WAT G | 206 | 50.00 | | | |
| HETATM | | OH2 | WAT G | 207 | 68.07 | 8 -16.236 | 83.621 | 1.00 29.70 |
| | | OH2 | WAT G | | 24.39 | 5 -4.134 | 111.635 | 1.00 50.82 |
| HETATM | 0433 | | | | | 4 2 664 | 114.289 | 1.00 44.49 |
| HETATM | 6234 | | WAT G | | 53.38 | | | |
| HETATM | 6235 | OH2 | WAT G | 210 | 60.12 | 0 -9.482 | 94.788 | 1.00 31.97 |
| HEIM TO | 6236 | | WAT G | | 23.40 | 5 17 472 | 111.744 | 1.00 44.97 |
| HETATM | 6236 | | | | | | | 1.00 59.14 |
| HETATM | 6237 | | WAT G | | 46.21 | | | |
| HETATM | | OH2 | WAT G | 213 | 29.75 | 4 6:983 | 97.109 | 1.00 41.78 |
| HETATM | 6220 | | WAT G | | 46.82 | 0 -0.465 | 55.181 | 1.00 41.02 |
| HETATM | 0233 | | | | 59.14 | | 124.775 | 1.00 38.42 |
| HETATM | 6240 | | WAT G | | | | | 1.00 32.50 |
| HETATM | 6241 | OH2 | WAT G | 216 | 42.67 | | | |
| HETATM | | OH2 | WAT G | 217 | 55.00 | 9 ~7.248 | 98.186 | 1.00 56.50 |
| | | | | | 63.36 | 1 -8 209 | 109.653 | 1.00 49.66 |
| HETATM | 6243 | | WAT G | | | | | 1.00 50.91 |
| HETATM | 6244 | | WAT G | | 66.58 | | | |
| HETATM | | OH2 | WAT G | 220 | 44.62 | 72.583 | 93.919 | 1.00 36.99 |
| | | | WAT G | | 24.47 | | | 1.00 47.24 |
| HETATM | 0240 | | | | | | | 1.00 50.43 |
| HETATM | 6247 | | WAT G | | 76.91 | 3 -1.111 | | |
| HETATM | | OH2 | WAT G | 223 | 32.78 | | 129.136 | 1.00 42.47 |
| | | | WAT G | | 73.73 | 1 -16.880 | 88.817 | 1.00 46.69 |
| HETATM | 0247 | | | | 78.56 | | | 1.00 43.17 |
| HETATM | 6250 | OHI | WAT G | | | | | 1.00 35.84 |
| HETATM | 6251 | OH. | WAT G | 226 | 45.68 | | | |
| HETATM | 6252 | OHL | WAT G | 227 | 38.26 | 3 15.236 | 84.711 | 1.00 42.39 |
| METATE | 6052 | G113 | WAT G | | 38.93 | 3 35 224 | 108.488 | 1.00 52.23 |
| HETATM | りとうう | UMZ | WAL G | 440 | | | | |
| 1144 | | | | | | F 44 020 | | 1 00 46 56 |
| HETATM | 6254 | OH2 | WAT G | 229 | 33.75 | 5 14.939 | 70.228 | 1.00 46.56 |
| HETATM | 6254 | OH2 | WAT G | 229 | 33.75 51.52 | 5 14.939 1 34.184 | 70.228 100.859 | 1.00 52.96 |
| HETATM HETATM | 6254 6255 | OH2 OH2 | WAT G | 229 230 | 51.52 | 1 34.184 | 70.228 | 1.00 52.96 |
| HETATM HETATM HETATM | 6254 6255 6256 | OH2 OH2 OH2 | WAT G WAT G | 229 230 231 | 51.52 34.14 | 1 34.184 0 0.565 | 70.228 100.859 63.039 | 1.00 52.96 1.00 31.02 |
| HETATM HETATM HETATM | 6254 6255 6256 | OH2 OH2 OH2 OH2 | WAT G WAT G WAT G | 229 230 231 232 | 51.52 34.14 37.27 | 1 34.184 0 0.565 7 13.977 | 70.228 100.859 63.039 81.662 | 1.00 52.96 1.00 31.02 1.00 39.83 |
| HETATM HETATM HETATM HETATM | 6254 6255 6256 6257 | OH2 OH2 OH2 OH2 | WAT G WAT G WAT G | 229 230 231 232 | 51.52 34.14 | 1 34.184 0 0.565 7 13.977 | 70.228 100.859 63.039 81.662 93.216 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 |
| HETATM HETATM HETATM HETATM HETATM | 6254 6255 6256 6257 6258 | OH2 OH2 OH2 OH2 OH2 | WAT G WAT G WAT G WAT G | 229 230 231 232 233 | 51.52 34.14 37.27 57.30 | 1 34.184 0 0.565 7 13.977 7 5.947 | 70.228 100.859 63.039 81.662 93.216 | 1.00 52.96 1.00 31.02 1.00 39.83 |
| HETATM HETATM HETATM HETATM HETATM HETATM | 6254 6255 6256 6257 6258 6259 | OH2 OH2 OH2 OH2 OH2 OH2 | WAT G WAT G WAT G WAT G WAT G | 229 230 231 232 233 234 | 51.52 34.14 37.27 57.30 31.71 | 34.184 0 0.565 7 13.977 7 5.947 .8 16.820 | 70.228 100.859 63.039 81.662 93.216 125.707 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 |
| HETATM HETATM HETATM HETATM HETATM HETATM HETATM | 6254 6255 6256 6257 6258 6259 6260 | OH2 OH2 OH2 OH2 OH2 OH2 | WAT G WAT G WAT G WAT G WAT G WAT G | 229 230 231 232 233 234 235 | 51.52 34.14 37.27 57.30 31.71 60.62 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 51.02 |
| HETATM HETATM HETATM HETATM HETATM HETATM HETATM | 6254 6255 6256 6257 6258 6259 6260 | OH2 OH2 OH2 OH2 OH2 OH2 | WAT G WAT G WAT G WAT G WAT G WAT G | 229 230 231 232 233 234 235 | 51.52 34.14 37.23 57.30 31.71 60.62 44.35 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 4 31.119 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 51.02 1.00 57.50 |
| HETATM HETATM HETATM HETATM HETATM HETATM HETATM HETATM HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G WAT G WAT G WAT G WAT G WAT G | 229 230 231 232 233 234 235 236 | 51.52 34.14 37.23 57.30 31.71 60.62 44.35 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 4 31.119 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 51.02 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 | 51.52 34.14 37.27 57.30 31.71 60.62 44.35 68.45 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 14 31.119 17 4.267 18 1.072 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 38.65 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 6263 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 | 51.52 34.14 37.27 57.30 31.77 60.62 44.35 68.45 27.83 | 1 34.184 0 0.565 7 13.977 7 5.947 16.820 14 31.119 17 4.267 14 1.072 16 6.773 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 38.65 1.00 44.95 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 6263 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 | 51.52 34.14 37.27 57.30 31.73 60.64 44.35 68.45 27.83 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 31.112 14 267 14 1.072 16 6.773 13 23.344 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 51.02 1.00 57.50 1.00 38.65 1.00 44.95 1.00 42.95 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 6263 6264 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 | 51.52 34.14 37.27 57.30 31.73 60.64 44.35 68.45 27.83 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 31.112 14 267 14 1.072 16 6.773 13 23.344 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 51.02 1.00 57.50 1.00 38.65 1.00 42.95 1.00 42.95 1.00 45.78 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 6263 6264 6265 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 240 | 51.52 34.14 37.27 57.30 31.73 60.62 44.35 68.45 27.83 - 54.93 34.07 | 1 34.184 0 0.565 7 13.977 7 5.947 8 16.820 31.11 6 1.072 6 6.773 13 23.344 12 -15.271 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 51.02 1.00 57.50 1.00 38.65 1.00 42.95 1.00 42.95 1.00 45.78 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 6263 6264 6265 6266 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 240 241 | 51.52 34.14 37.27 57.30 31.73 60.63 44.35 68.43 27.83 - 54.93 34.07 | 1 34.184 0 0.565 7 13.977 18.947 18.16.820 14.31.119 17.4.267 18.6.6.773 18.3.344 18.3.344 18.3.344 18.3.344 18.3.344 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 61.973 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 57.50 1.00 42.95 1.00 42.95 1.00 38.91 |
| HETATM | 6254 6255 6256 6257 6258 6259 6260 6261 6262 6263 6264 6265 6266 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 240 241 242 | 51.52 34.14 37.27 57.30 31.77 60.62 44.35 68.45 27.83 - 54.93 34.96 | 1 34.184 0 0.565 7 13.977 18 16.820 14 31.119 17 4.267 18 16.773 18 16 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 61.973 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 57.50 1.00 44.95 1.00 42.95 1.00 45.78 1.00 38.91 1.00 44.85 |
| HETATM | 6254 6255 6256 6257 6258 6259 6261 6263 6264 6265 6266 6267 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 240 241 242 | 51.52 34.14 37.27 57.30 31.77 60.62 44.35 68.45 27.83 - 54.93 34.96 | 1 34.184 0 0.565 7 13.977 16.82 14 31.119 17 4.267 18 16.773 19 23.344 10 -15.271 10 189 10 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 61.973 127.376 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 38.65 1.00 44.95 1.00 42.95 1.00 45.78 1.00 38.91 1.00 44.85 1.00 38.32 |
| HETATM | 6254 6255 6256 6257 6259 6261 6262 6263 6264 6265 6267 6268 | OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 | 51.52 34.14 37.27 57.30 31.77 60.62 44.35 68.45 27.83 - 54.93 34.94 29.66 49.53 | 1 34.184 0 0.565 7 13.977 16.82 14 31.119 17 4.267 18 16.773 19 23.344 10 -15.271 10 189 10 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 61.973 127.376 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 38.65 1.00 44.95 1.00 42.95 1.00 45.78 1.00 38.91 1.00 44.85 1.00 38.32 |
| HETATM | 6254 6255 6256 6257 6259 6261 6263 6264 6265 6267 6268 6268 6268 | OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 240 241 242 243 244 | 51.52 34.14 37.27 57.30 31.77 60.62 44.35 68.45 27.83 - 54.93 34.07 35.96 49.55 | 1 34.184 0 0.565 7 13.977 7 5.947 16.820 14 31.119 17 4.267 18 1.072 18 23.344 2 -15.271 1.059 18 -10.150 19 9.773 | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 61.973 127.376 113.501 96.696 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 38.65 1.00 44.95 1.00 42.95 1.00 45.78 1.00 48.83 1.00 38.32 1.00 48.83 |
| HETATM | 6254 6255 6256 6257 6259 6261 6263 6264 6265 6267 6268 6268 6268 | OH2 | WAT G | 229 230 231 232 233 234 235 236 237 238 240 241 242 243 244 | 51.52 34.14 37.27 57.30 31.77 60.62 44.35 68.45 27.83 - 54.93 34.94 29.66 49.53 | 1 34.184 0 0.565 7 13.977 16.82 14.267 14.267 16.6773 13.344 12.672 13.344 12.673 13.344 14.267 15.271 16.59 17.36 18.371 18. | 70.228 100.859 63.039 81.662 93.216 125.707 110.067 94.916 70.111 79.253 81.087 71.579 61.973 127.376 113.501 96.696 | 1.00 52.96 1.00 31.02 1.00 39.83 1.00 28.55 1.00 53.16 1.00 57.50 1.00 38.65 1.00 44.95 1.00 42.95 1.00 45.78 1.00 48.91 1.00 38.91 1.00 44.85 1.00 38.32 1.00 48.83 |

| HETATM 6271 OH2 WAT G 246 | 50.248 -5.552 102.815 1.00 43.23 |
|---------------------------------------|--|
| HETATM 6272 OH2 WAT G 247 | |
| | 47.966 21.564 79.321 1.00 36.79 |
| HETATM 6273 OH2 WAT G 248 | 62.507 20.866 108.414 1.00 35.30 |
| HETATM 6274 OH2 WAT G 249 | |
| | 2,125 |
| HETATM 6275 OH2 WAT G 250 | 38.406 9.828 67.749 1.00 33.71 |
| HETATM 6276 OH2 WAT G 251 | 35.304 -6.179 66.319 1.00 36.23 |
| | |
| | 39.218 -12.667 85.010 1.00 36.17 |
| HETATM 6278 OH2 WAT G 253 | 56.350 5.089 97.225 1.00 46.38 |
| HETATM 6279 OH2 WAT G 254 | 20.50 |
| REIAIN 02/3 ONZ WAI G 254 | 69.850 3.406 122.119 1.00 55.07 |
| HETATM 6280 OH2 WAT G 255 | 75.703 2.630 128.600 1.00 30.64 |
| | |
| | 32.019 -12.973 113.965 1.00 34.48 |
| HETATM 6282 OH2 WAT G 257 | 54.081 3.421 56.994 1.00 39.11 |
| · HETATM 6283 OH2 WAT G 258 | |
| | |
| | 45.040 0.301 95.449 1.00 36.57 |
| HETATM 6285 OH2 WAT G 260 | 39.815 21.460 128.855 1.00 40.10 |
| HETATM 6286 OH2 WAT G 261 | |
| MEIRIN 0200 OHZ WAI G ZOI | 28.763 10.408 93.790 1.00 44.39 |
| HETATM 6287 OH2 WAT G 262 | 49.668 -12.050 60.539 1.00 50.89 |
| HETATM 6288 OH2 WAT G 263 | |
| HEREN COOL ONE WAT O 200 | |
| HETATM 6289 OH2 WAT G 264 | 75.183 13.021 128.124 1.00 50.42 |
| HETATM 6290 OH2 WAT G 265 | |
| | |
| HETATM 6291 OH2 WAT G 266 | 68.708 13.973 70.958 1.00 37.90 |
| HETATM 6292 OH2 WAT G 267 | 71.504 12.997 130.029 1.00 38.78 |
| HETATM 6293 OH2 WAT G 268 | |
| | |
| HETATM 6294 OH2 WAT G 269 | 65.973 12.195 79.625 1.00 51.68 |
| HETATM 6295 OH2 WAT G 270 | |
| · · · · · · · · · · · · · · · · · · · | |
| HETATM 6296 OH2 WAT G 271. | 44.433 -17.578 62.734 1.00 49.33 |
| HETATM 6297 OH2 WAT G 272 | 26.917 15.038 89,067 1.00 38.07 |
| HETATM 6298 OH2 WAT G 273 | |
| | 63.380 -5.416 126.550 1.00 41.73 |
| HETATM 6299 OH2 WAT G 274 | 63.360 -5.356 95.641 1.00 37.54 |
| HETATM 6300 OH2 WAT G 275 | 11 11 21 21 21 21 21 21 21 21 21 21 21 2 |
| | |
| HETATM 6301 OH2 WAT G 276 | 26.406 25.831 117.328 1.00 48.37 |
| HETATM 6302 OH2 WAT G 277 | 41.893 -10.251 98.201 1.00 46.36 |
| HETATM 6303 OH2 WAT G 278 | |
| METATA 0303 ONZ WAI G 2/8 | 30.343 -6.507 117.764 1.00 49.87 |
| HETATM 6304 OH2 WAT G 279. | 45.135 32:419 111.056 1.00 43.93 |
| HETATM 6305 OH2 WAT G 280 | |
| | |
| HETATM 6306 OH2 WAT G 281 | 60.428 13.652 105.130 1.00 31.10 |
| HETATM 6307 OH2 WAT G 282 | 30.342 2.204 70.246 1.00 45.19 |
| HETATM 6308 OH2 WAT G 283 | |
| | 60.358 15.921 127.736 1.00 33.17 |
| HETATM 6309 OH2 WAT G 284 | 64.193 3.421 62.117 1.00 45.81 |
| HETATM 6310 OH2 WAT G 285 | 45.468 6.113 105.853 1.00 48.98 |
| | |
| HETATM 6311 OH2 WAT G 286 | 47.514 3.808 98.279 1.00 46.45 |
| HETATM 6312 OH2 WAT G 287 | 72.144 -6.345 77.930 1.00 40.04 |
| HETATM 6313 OH2 WAT G 288 | |
| | |
| HETATM 6314 OH2 WAT G 289 | 48.982 13.297 65.822 1.00 46.98 |
| HETATM 6315 OH2 WAT G 290 | 41.171 34.107 115.807 1.00 51.76 |
| HETATM 6316 CH2 WAT G 291 | |
| | 36.494 37.195 104.170 1.00 44.27 |
| HETATM 6317 OH2 WAT G 292 | 48.580 23.117 85.456 1.00 40.96 |
| HETATM 6318 OH2 WAT G 293 | |
| | |
| HETATM 6319 OH2 WAT G 294 | 61.720 11.077 89.427 1.00 41.21 |
| HETATM 6320 OH2 WAT G 295 | 43.313 -18.552 114.112 1.00 42.32 |
| HETATM 6321 OH2 WAT G 296 | |
| ABIATH USEL UNE WAT G 296 | 53.001 -6.305 129.052 1.00 37.41 |
| HETATM 6322 OH2 WAT G 297 | 70.258 24.928 82.843 1.00 48.09 |
| HETATM 6323 OH2 WAT G 298 | 77.493 0.940 130.507 1.00 51.77 |
| | |
| HETATM 6324 OH2 WAT G 299 | 32.233 12.182 83.028 1.00 53.51 |
| HETATM 6325 OH2 WAT G 300 | 40.666 12.878 65.747 1.00 46.49 |
| HETATM 6326 OH2 WAT G 301 | |
| | 50.977 12.831 114.597 1.00 48.51 |
| HETATM 6327 OH2 WAT G 302 | 54.236 3.817 92.196 1.00 41.15 |
| HETATM 6328 CH2 WAT G 303 | 59.527 -1.343 107.471 1.00 36.71 |
| | |
| HETATM 6329 OH2 WAT G 304 | 70.331 3.940 89.312 1.00 47.70 |
| HETATM 6330 CH2 WAT G 305 | 60.626 6.969 127.780 1.00 41.96 |
| HETATM 6331 OH2 WAT G 306 | |
| | |
| HETATM 6332 OH2 WAT G 307 | 58.886 16.514 99.413 1.00 53.60 |
| HETATM 6333 OH2 WAT G 308 | 67.617 -1.589 96,570 1.00 40.36 |
| · | |
| | 35.868 -10.936 98.849 1.00 48.80 |
| HETATM 6335 OH2 WAT G 310 | 45.576 25.388 131.914 1.00 48.99 |
| HETATM 6336 CH2 WAT G 311 | 37.583 -6.243 64.257 1.00 37.06 |
| MI G off | |
| | |

Figure 18-97

| | | | | | | | | | | 45 00 |
|--|------|------|-------|-----|---|--------|---------|---------|------|-------|
| HETATM | 6337 | OH2 | WAT G | 312 | | 66.759 | 16.408 | 94.600 | | 45.07 |
| HETATM | | OH2 | WAT G | 313 | | 24.142 | 11.212 | 113.340 | 1.00 | 52.23 |
| | | | | | | | 16.702 | 64.230 | | 39.88 |
| HETATM | | | WAT G | | | 69.409 | | | | |
| HETATM | 6340 | OH2 | WAT G | 315 | | 22.064 | 24.858 | 115.328 | | 50.23 |
| HETATM | | OH2 | WAT G | 316 | | 50.171 | 9.551 | 100.345 | 1.00 | 37.32 |
| | | | | | | | 31.302 | | | 44.78 |
| HETATM | 6342 | OH2 | WAT G | 311 | | 55.104 | | | | |
| HETATM | 6343 | OH2 | WAT G | 318 | | 65.333 | -10.105 | 95.866 | 1.00 | 44.21 |
| 117711111 | 6344 | | WAT G | | | 31.415 | | 128.127 | 1.00 | 41.95 |
| HETATM | 0244 | | | | | | | | | 44.79 |
| HETATM | 6345 | | WAT G | | | 37.423 | 13.143 | 88.069 | | |
| HETATM | 6346 | OH2. | WAT G | 321 | | 43.619 | 14.292 | 96.509 | 1.00 | 54.69 |
| | | | WAT G | | | 68.048 | 14 555 | 126.016 | 1.00 | 42.75 |
| HETATM | | | | | | | | | | 37.06 |
| HETATM | 6348 | OH2 | WAT G | 323 | | 34.778 | -2.509 | - | | - |
| HETATM | | OH2 | WAT G | 324 | - | 27.972 | 18.144 | 103.841 | 1.00 | 47.34 |
| | | | WAT G | | | 53.550 | 23.610 | 97.592 | 1.00 | 38.03 |
| HETATM | | | | | | | | | | |
| HETATM | 6351 | OH2 | WAT G | 326 | | 33.776 | 4.171 | 103.451 | | 50.60 |
| HETATM | 6352 | OH2 | WAT G | 327 | | 37.862 | 35.632 | 114.870 | 1.00 | 48.34 |
| HEIMIN | 6352 | | | | | 50.893 | 14.612 | 93.478 | 1 00 | 38.77 |
| HETATM | 6353 | | WAT G | | | | | | | |
| HETATM | 6354 | OH2 | WAT G | 329 | | | -20.913 | 86.137 | | 47.69 |
| HETATM | | OH2 | WAT G | 330 | | 50.310 | -23.133 | 74.502 | 1.00 | 41.94 |
| | | | | | | | 7.269 | 60.583 | 1 00 | 54.93 |
| HETATM | | | WAT G | | | 41.520 | | | | |
| HETATM | 6357 | OH2 | WAT G | 332 | | 75.879 | 13.737 | 106.089 | | 44.65 |
| HETATM | 6358 | OH2 | WAT G | 333 | | 51.923 | 9.027 | 138.493 | 1.00 | 41.08 |
| | | | | | | | 27.611 | 79.363 | 1 00 | 39.05 |
| HETATM | | | WAT G | | | 49.511 | | | | |
| HETATM | 6360 | OH2 | WAT G | 335 | | 69.385 | 0.852 | 110.192 | _ | 41.42 |
| HETATM | | OH2 | WAT G | 336 | | 40.952 | 2.479 | 101.880 | 1.00 | 42.50 |
| | | | | | | 32.998 | | 103.784 | 1.00 | 54.22 |
| HETATM | 6362 | | WAT G | | | | | | | |
| HETATM | 6363 | OH2 | WAT G | 338 | | 54.366 | 15.261 | 136.205 | | 52.69 |
| HETATM | | OH2 | WAT G | 339 | | 35.674 | 13.727 | 89.792 | 1.00 | 35.83 |
| | | | | | | | -21.361 | 87.138 | 1.00 | 46.26 |
| HETATM | | | WAT G | | | | -21.301 | | | |
| HETATM | 6366 | OH2 | WAT G | 341 | | 72.053 | 4.708 | 131.550 | | 45.27 |
| HETATM | 6367 | OH2 | WAT G | 342 | • | 28.072 | -1.358 | 70.419 | 1.00 | 34.92 |
| HETAIN | 6367 | | | | | 23.611 | -3.981 | 76.422 | 1.00 | 52.99 |
| HETATM | 6368 | | WAT G | | | | | | | 58.16 |
| HETATM | 6369 | OH2 | WAT G | 344 | | 53.684 | | 122.150 | | |
| HETATM | | OH2 | WAT G | 345 | | 30.624 | -6:528 | 125.556 | 1.00 | 34.71 |
| | | | | | | 27.870 | | 113.997 | 1.00 | 44.91 |
| HETATM | 63/1 | | WAT G | | | | | | | 55.34 |
| HETATM | 6372 | OH2 | WAT G | 347 | | 31.903 | | 116.327 | | |
| HETATM | 6373 | OH2 | WAT G | 348 | | 71.763 | 15.094 | 63.739 | 1.00 | 48.99 |
| | | | WAT G | | | 25.258 | -2 536 | 114.760 | 1.00 | 37.19 |
| HETATM | 63/4 | | | | | | | | | 42.32 |
| HETATM | 6375 | OH2 | WAT G | 350 | | 43.765 | 12.162 | 78.143 | | |
| HETATM | 6376 | OH2 | WAT G | 351 | | 32.452 | 5.338 | 73.909 | 1.00 | 33.70 |
| HEIMIN | 6377 | | | | | 52.896 | -5 770 | 101.894 | 1.00 | 46.40 |
| HETATM | 63// | | WAT G | | | | | | | 34.62 |
| HETATM | 6378 | OH2 | WAT G | 353 | | 47.968 | 4.242 | 115.852 | | |
| HETATM | 6379 | OH2 | WAT G | 354 | | 38.561 | -9.302 | 90.596 | | 49.80 |
| REIMIN | 6300 | | WAT G | | | 63.791 | 17.454 | 74.354 | 1.00 | 56.40 |
| HETATM | 0360 | | | | | | | | | 50.00 |
| HETATM | 6381 | OHZ | _ | 356 | | 41.360 | | 133.760 | | |
| HETATM | 6382 | OH2 | WAT G | 357 | | 42.467 | ~7.937 | 122.328 | | 38.01 |
| ************************************** | 6303 | | | 358 | | 50.890 | 0.362 | 116.668 | 1.00 | 39.26 |
| HETATM | 0202 | | | | | E4 317 | | 67.865 | | 55.18 |
| HETATM | 6384 | | | 359 | | | -23.881 | | | |
| HETATM | 6385 | OH2 | WAT G | 360 | | 64.959 | | 105.032 | | 38.83 |
| HETATM | 6386 | | WAT G | | | 58,113 | -19.846 | 82.288 | 1.00 | 38.60 |
| HETATM | 0000 | | | | | | -1.140 | | | 31.47 |
| HETATM | 6387 | | WAT G | | | 42.245 | | | | |
| HETATM | 6388 | OH2 | WAT G | 363 | | 73.552 | 17.770 | 125.885 | | 54.89 |
| DESTRUCTION OF THE PARTY OF THE | 6300 | | | 364 | | 68.769 | 15.898 | 106.810 | 1.00 | 45.53 |
| HETATM | 0003 | | | | | | | 78.866 | | 45.15 |
| HETATM | 6390 | | WAT G | | | 37.543 | 19.031 | | | |
| HETATM | 6391 | OH2 | WAT G | 366 | | 55.583 | 6.906 | 95.087 | | 44.99 |
| Division and | 6302 | | WAT G | | | 41.284 | 9.699 | 78.250 | 1.00 | 36.58 |
| HETATM | 0334 | | | | | | | 126.362 | | 46.60 |
| HETATM | 6393 | | WAT G | | | 25.203 | 5.332 | | | |
| HETATM | 6394 | OH2 | WAT G | 369 | | 74.742 | -5.006 | 95.104 | | 47.85 |
| DEAD IN | 6305 | | WAT G | | | 70.349 | 19.871 | 69.925 | 1.00 | 51.46 |
| HETATM | 0333 | | | | | | | 94.720 | | 38.66 |
| HETATM | 6396 | | WAT G | | | 42.936 | 20.631 | | | |
| HETATM | 6397 | OH2 | WAT G | 372 | | 34.162 | -16.114 | 114.141 | | 44.01 |
| HEIMIN | 6300 | | WAT G | | | 33.863 | 16.838 | 100.275 | 1.00 | 44.66 |
| HETATM | 0000 | | | | | | 12.569 | 86.140 | | 43.89 |
| HETATM | 6399 | OHZ | WAT G | 374 | | 21.613 | 14.509 | | 1.00 | E2 E2 |
| HETATM | 6400 | OH2 | WAT G | 375 | | 35.751 | -13.302 | 100.583 | 1.00 | 53:53 |
| PPINIT | 5401 | | WAT G | | | 70.095 | 13.395 | 117.505 | 1.00 | 52.02 |
| HETATM | 04UI | | | | | | | | 1 00 | 46.47 |
| HETATM | 6402 | OHZ | WAT G | 377 | | 41.853 | TA'TOR | 131.799 | 1.00 | =0.7/ |
| | | · | | | | | | | | |
| | | | | | | | | | | |

| HETATM 6403 OH2 WAT G 378 | 55.780 -14.986 65.487 1.00 49.09 |
|--|--|
| HETATM 6404 OH2 WAT G 379 | 40.990 21.205 91.611 1.00 41.02 |
| HETATM 6405 OH2 WAT G 380 | 48.157 1.057 116.992 1.00 44.84 |
| HETATM 6406 OH2 WAT G 381 HETATM 6407 OH2 WAT G 382 | 37.954 -6.221 128.334 1.00 37.09 |
| | 30.221 27.743 109.194 1.00 39.92 |
| HETATM 6408 OH2 WAT G 383 HETATM 6409 OH2 WAT G 384 | 49.926 -12.826 118.421 1.00 58.95 |
| HETATM 6410 OH2 WAT G 385 | 42.435 -17.636 81.477 1.00 48.47 |
| HETATM 6411 OH2 WAT G 386 | 58.226 -25.990 71.378 1.00 48.18 40.495 17.944 128.741 1.00 43.82 |
| HETATM 6412 OH2 WAT G 387 | |
| HETATM 6413 OH2 WAT G 388 | |
| HETATM 6414 OH2 WAT G 389 | 47.277 2.559 100.509 1.00 43.00 38.862 9.112 102.620 1.00 31.70 |
| HETATM 6415 OH2 WAT G 390. | 71.652 14.568 105.167 1.00 49.63 |
| HETATM 6416 OH2 WAT G 391 | 68.554 -10.518 73.331 1.00 38 16 |
| HETATM 6417 OH2 WAT G 392 | 70.496 -16.160 84.425 1.00 32.16 |
| HETATM 6418 OH2 WAT G 393 HETATM 6419 OH2 WAT G 394 | 44.698 -24.950 75.603 1.00 43.38 |
| HETATM 6419 OH2 WAT G 394 HETATM 6420 OH2 WAT G 395 | 56.172 15.369 55.027 1.00 47.44 |
| HETATM 6421 OH2 WAT G 396 | 46.150 -9.441 99.999 1.00 47.98 |
| HETATM 6422 OH2 WAT G 397 | 26.892 -8.356 89.057 1.00 34.99 31.737 14.380 90.395 1.00 50 78 |
| HETATM 6423 OH2 WAT G 398 | 2.00 30.70 |
| HETATM 6424 OH2 WAT G 399 | 36.261 -13.824 62.777 1.00 50.86 37.312 15.242 134.977 1.00 43.57 |
| HETATM 6425 OH2 WAT G 400 | 33.728 13.773 126.419 1.00 57.13 |
| HETATM 6426 OH2 WAT G 401 | 45.269 27.937 130.311 1.00 49 55 |
| HETATM 6427 OH2 WAT G 402 | 44.887 -17.414 111.508 1.00 54.29 |
| HETATM 6428 OH2 WAT G 403 | 68.928 0.455 136.711 1.00 49.90 |
| HETATM 6429 OH2 WAT G 404 HETATM 6430 OH2 WAT G 405 | 43.271 -21.571 64.425 1.00 48.61 |
| HETATM 6430 OH2 WAT G 405 HETATM 6431 OH2 WAT G 406 | 24.243 -4.781 108.590 1.00 51.05 |
| HETATM 6432 OH2 WAT G 407 | 54.828 5.311 59.009 1.00 43.43 53.460 27.992 124.076 1.00 47.83 |
| | 53.460 27.992 124.076 1.00 47.83 70.833 -18.390 85.386 1.00 49.26 |
| HETATM 6434 OH2 WAT G 409 | 71 497 15 297 117 071 1 00 24 50 |
| HETATM 6435 OH2 WAT G 410 | 36.407 -18.480 110.466 1.00 55.43 |
| HETATM 6436 OH2 WAT G 411 | 26.220 -9.551 78.158 1.00 47.69 |
| HETATM 6437 OH2 WAT G 412 HETATM 6438 OH2 WAT G 413 | 52.319 26.326 82.038 1.00 42.00 |
| HETATM 6438 OH2 WAT G 413 HETATM 6439 OH2 WAT G 414 | 76.173 14.097 122.253 1.00 44.90 58.379 6.335 123.024 1.00 54.61 |
| HETATM 6440 OH2 WAT G 415 | |
| HETATM 6441 OH2 WAT G 416 | 72.162 -16.705 82.719 1.00 50.63 63.557 26.152 65.944 1.00 39.83 |
| HETATM 6442 OH2 WAT G 417 | 38.935 23.070 122.742 1.00 52.57 |
| HETATM 6443 OH2 WAT G 418 | 55.256 -10.714 124.501 1.00 42.38 |
| HETATM 6444 OH2 WAT G 419 | 55.443 -9.037 110.170 1.00 46.47 |
| HETATM 6445 OH2 WAT G 420 HETATM 6446 OH2 WAT G 421 | 73.873 16.578 123.288 1.00 46.54 |
| HETATM 6447 CH2 WAT G 421 | 74.426 12.663 117.527 1.00 43.62 |
| HETATM 6448 OH2 WAT G 423 | 52.374 -0.368 51.502 1.00 56.99 60.339 20.215 84.713 1.00 36.27 |
| HETATM 6449 OH2 WAT G 424 | 60.339 20.215 84.713 1.00 36.27 48.308 1.354 54.561 1.00 38.53 |
| HETATM 6450 OH2 WAT G 425 | 61.757 21.606 115.976 1.00 61.09 |
| HETATM 6451 OH2 WAT G 426 | 33.222 -14.916 119.528 1.00 51.12 |
| HETATM 6452 OH2 WAT G 427 | 47.477 3.359 112.298 1.00 46.10 |
| HETATM 6453 OH2 WAT G 428 HETATM 6454 OH2 WAT G 429 | 39.909 2.272 138.388 1.00 35.33 |
| HETATM 6454 OH2 WAT G 429 HETATM 6455 OH2 WAT G 430 | 57.829 15.336 126.262 1.00 62.59 |
| HETATM 6456 OH2 WAT G 431 | 48.917 -5.857 119.191 1.00 51.45 44.139 -3.812 132.964 1.00 44.91 |
| HETATM 6457 OH2 WAT G 432 | 44.139 -3.812 132.964 1.00 44.91 38.885 18.594 95.398 1.00 50.23 |
| HETATM 6458 OH2 WAT G 433 | 52.628 -7.064 55.271 1.00 38.96 |
| HETATM 6459 OH2 WAT G 434 | 60.644 -0.731 101.129 1.00 47.30 |
| HETATM 6460 OH2 WAT G 435 | 64.772 5.808 71.942 1.00 50.81 |
| HETATM 6461 OH2 WAT G 436 | 39.571 16.705 80.180 1.00 34.07 |
| HETATM 6462 OH2 WAT G 437 HETATM 6463 OH2 WAT G 438 | 32.791 -0.551 65.371 1.00 41.40 |
| HETATM 6464 OH2 WAT G 438 | 58.318 -7.989 60.087 1.00 46.94 |
| HETATM 6465 OH2 WAT G 440 | 26.982 5.474 120.408 1.00 46.28 72.138 1.233 90.050 1.00 50.13 |
| HETATM 6466 OH2 WAT G 441 | 29.494 10.971 118.393 1.00 56.30 |
| HETATM 6467 OH2 WAT G 442 | 69.232 5.594 113.941 1.00 58.17 |
| HETATM 6466 OH2 WAT G 443 | 61.459 11.576 71.140 1.00 61.67 |
| Olinasan- | • · |
| THEFT | CHIFFY AND TOO |

WO 01/018045 PCT/US00/24700

215/263 Figure 18-99

| HETATM | 6469 | он2 | WAT | G | 444 | 59. | 592 | 2.195 | 58.518 | | 42.66 |
|--------------|------|-----|------|---|-----|-------|-----|---------|---------|------|-------|
| HETATM | 6470 | OH2 | TAW_ | G | 445 | 47. | 407 | 6.152 | 111.310 | | 45.14 |
| HETATM | 6471 | OH2 | WAT | G | 446 | 36. | 254 | 18.203 | 99.930 | | 44.76 |
| HETATM | 6472 | OH2 | WAT | G | 447 | 49. | 525 | 32.050 | 116.235 | 1.00 | 47.72 |
| HETATM | | OH2 | WAT | G | 448 | 21. | 801 | -5.358 | 81.109 | 1.00 | 42.07 |
| HETATM | | | WAT | | | 52. | 131 | ~14.007 | 95.380 | 1.00 | 40.76 |
| HETATM | | | WAT | _ | | 39. | 712 | -19.983 | 72.499 | 1.00 | 51.69 |
| HETATM | | | WAT | _ | | 67. | 651 | 5.620 | 67.102 | 1.00 | 42.38 |
| HETATM | - | | WAT | | | 77. | 344 | 1.313 | 79,207 | 1.00 | 63.64 |
| HETATM | | | WAT | | | | | -29.426 | 86.187 | 1.00 | 44.98 |
| | | | WAT | - | | | | -11.004 | 98.104 | 1.00 | 49.12 |
| HETATM | | | WAT | - | | • • • | 456 | | 129.510 | | 61.60 |
| HETATM | - | | | | | | | -14.790 | 68.028 | | 40.08 |
| HETATM | | | WAT | | | | 732 | | 94.924 | | 58.32 |
| TATALAN TIME | | | | | | | | | | | |

Figure 19-1

| | Resid | ue #X | Y | Z | D 0 | |
|--------------|----------------------------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1 CE ALA A 2 | 45.86 | | | B Segment 1.00 57.10 | |
| ATOM | 2 C ALA A 2 | 46.76 | | | | AAAA |
| MOTA | 3 0 ALA A 2 | 46.33 | | | | AAAA |
| ATOM | 4 :: ALA A 2 | 48.28 | | | | AAAA |
| MOTA | 5 CA ALA A 2 | 47.06 | | | | AAAA |
| ATOM | 6 N LYSA 3 | 46.97 | | | | AAAA |
| ATCM | 7 CA LYS A 3 | 46.72 | | | | AAAA AAAA |
| ATOM | 8 CE LYS A 3 | 47.81 | 5 39.778 | 69.939 | 1.00 53.86 | AAAA |
| MOTA | 9 CG LYS A 3 | 49.22 | 3 -39.876 | 70.490 | | AAAA |
| ATOM | 10 CD LYS A 3 | 50.25 | | | 1.00 57.84 | AAAA |
| ATOM | 11 CE LYS A 3 | 51.65 | | 69.957 | 1.00 58.89 | AAAA |
| ATOM | 12 NZ LYS A 3 | 52.643 | | | 1.00 59.33 | AAAA |
| ATOM | 13 C LYS A 3 | 45.393 | | 70.305 | 1.00 49.57 | . AAAA |
| ATOM | 14 0 LYS A 3 | 44.894 | | | 1.00 49.33 | AAAA |
| ATOM | 15 N VAL A 4 | 44.826 | | | 1.00 46.23 | AAAA |
| ATOM | 16 CA VAL A 4 | 43.561 | | _ | 1.00 42.51 | AAAA |
| ATOM ATOM | 17 CB VAL A 4 18 CG1 VAL A 4 | 42.543 | | | 1.00 42.26 | AAAA |
| ATOM | | 41.213 | | | 1.00 41.51 | AAAA |
| ATOM | 19 CG2 VAL A 4 20 C VAL A 4 | 42.401 | | | 1.00 42.00 | AAAA |
| ATOM | 21 0 VALA 4 | 43.918 | | 67.638 | 1.00 39.94 | AAAA |
| MOTA | 22 N LYS A 5 | 44.332 43.766 | | | 1.00 40.39 | AAAA |
| ATOM | 23 CA LYS A 5 | 44.142 | | 66.695 | 1.00 36.94 | AAAA |
| ATOM | 24 CB LYS A 5 | 45.179 | | | 1.00 34.10 | አጸጸሕ |
| ATOM | 25 CG LYS A 5 | 46.424 | | 64.846 65.698 | 1.00 35.02 | AAAA |
| ATOM | 26 CD LYS A 5 | 47.233 | | 65.652 | 1.00 34.07 | AAAA |
| MOTA | 27 CE LYS A 5 | 48.565 | | 66.333 | 1.00 33.44 1.00 32.38 | AAAA |
| MOTA | 28 NZ LYS A 5 | 49.372 | | 66.222 | 1.00 31.36 | AAAA |
| ATOM | 29 C LYS A 5 | 42.997 | | 64.333 | 1.00 31.38 | ሕሕሕ ሕሕA |
| ATOM | 30 0 LYS A 5 | 42.053 | | 64.466 | 1.00 31.74 | AAAA |
| ATOM | 31 H LEU A 6 | 43.090 | 41.142 | 63.326 | 1.00 28.60 | AAAA |
| ATOM | 32 CA LEU A 6 | 42.075 | 41.167 | 62.289 | 1.00 26.90 | AAAA |
| ATOM | 33 CB LEU A 6 | 41.530 | 42.580 | 62.067 | 1.00 26.43 | AAAA |
| ATOM | 34 CG LEU A 6 | 40.321 | 42.748 | 61.129 | 1.00 25.89 | AAAA |
| ATOM | 35 CD1 LEU A - 6 | 40.108 | 44.224 | 60.826 | 1.00 25.50 | AAAA |
| ATOM ATOM | 36 CD2 LEU A 6 37 C LEU A 6 | 40.550 | 42.032 | 59.828 | 1.00 26.64 | AAAA |
| ATOM | 37 C LEU A 6 38 C LEU A 6 | 42.818 | 40.701 | 61.049 | 1.00 25.74 | AAAA |
| ATOM | 39 N ILE A 7 | 43.877 | 41.226 | 60.717 | 1.00 24.60 | AAAA |
| ATOM | | 42.282 42.939 | 39.704 | 60.367 | 1.00 25.90 | AAAA |
| ATOM | 40 CA ELE A 7 41 CB ELE A 7 | 42.839 | 39.212 37.712 | 59.173 | 1.00 26.75 | AAAA |
| ATOM | 42 CG2 ILE A 7 | 43.474 | 37.712 | 59.089 57.783 | 1.00 26.58 1.00 27.88 | AAAA |
| ATOM | 42 CG2 ILE A 7 43 CG1 ILE A 7 | 43.528 | 37.116 | 60.310 | 1.00 27.02 | AAAA |
| ATOM | 44 CD1 TLE A 7 | 43.507 | 35.640 | 60.350 | 1.00 27.46 | AAAA |
| ATOM | 45 C' ILE A 7 | 42.339 | 39.814 | 57.929 | 1.00 25.70 | аааа аааа |
| ATOM | 46 0 ILE A 7 | 41.162 | 39.655 | 57.681 | 1.00 27.68 | AAAA |
| ATOM | 47 N GLY A 8 | 43.144 | 40.509 | 57.142 | 1.00 27.94 | AA A |
| atcm | 48 CA GLY A 8 | 42.598 | 41.110 | 55.944 | 1.00 29.78 | AA. A |
| ATOM | 49 C GLY A 8 | 43.587 | 41.789 | 55.027 | 1.00 30.38 | AAAA |
| ATOM | 50 0 GLY A 8 | 44.785 | 41.765 | 55.264 | 1.00 29.39 | AAAA |
| ATOM | 51 N THRA 9 | 43.051 | 42.395 | 53.971 | 1.00 31.84 | AAAA |
| ATCM | 52 CA THRA 9 | 43.832 | 43.106 | 52.962 | 1.00 32.41 | AAAA |
| ATCM | 53 CB THR A 9 54 CG1 THR A 9 | 44.606 | 42.112 | 52.064 | 1.00 31.12 | AAAA |
| atom atom | 54 CG1 THR A 9 55 CG2 THR A 9 | 45.324 | 42.825 | 51.053 | 1.00 30.74 | AAAA |
| ATOM | 56 C THR A 9 | 43.654 42.886 | 41.140 | 51.411 | 1.00 30.27 | AAAA |
| ATOM | 57 0 THR A 9 | 41.705 | 43.939 | 52.091 | 1.00 32.94 | AAAA |
| ATOM | 58 H LEUA 10 | 43.396 | 43.625 45.009 | 51.993 51.485 | 1.00 33.62 | AAAA |
| ATOM | 59 CA LEU A 10 | 42.573 | 45.840 | 50.611 | 1.00 33.20 | AAAA |
| ATOM | 60 CB LEU A 10 | 43.117 | 47.275 | 50.484 | 1.00 33.29 1.30 33.12 | AAAA |
| ATCM | 51 CG LEU A 10 | 43.142 | 48.245 | | 1.00 33.12 | AAAA |
| ATCM | 62 CD1 LEU A 10 | 41.743 | 48.386 | | 1.00 32.95 | AAAA |
| ATOM | 63 CD2 LEU A 10 | 44.126 | 47.734 | | 1.00 34.71 | AAAA |
| ATCM | 64 C LEU A 10 | 42.527 | | | 1.00 33.18 | AAAA AAAA |
| ATCM | 65 0 LEU A 10 | 41.876 | 45.768 | | 1.00 32.52 | AAAA |
| atom | 66 N ASP A 11 | 43.230 | | | 1.00 33.56 | AAAA |
| | | | _ | | | |

| | | | | | 42 240 | 43 400 | 17 716 | 1 00 34 34 | AAAA |
|--------|------|-----|--------|----|----------|--------|---------|------------|--------|
| MOTA | 67 | CA | ASP A | 11 | 43.240 | 43.489 | 47.716 | 1.00 34.24 | |
| MOTA | 68 | CB | ASP A | 11 | 44.393 | 42.499 | 47.607 | 1.00 35.81 | AAAA |
| | 69 | CG | ASP A | 11 | 45.739 | 43.190 | 47.604 | 1.00 37.57 | AAAA |
| MOTA | | | | | 45.890 | 44.178 | 46.855 | 1.00 37.95 | AAAA |
| MOTA | 70 | | ASP A | 11 | | | | 1.00 40.31 | AAAA |
| MOTA | 71 | OD2 | ASP A | 11 | 46.650 | 42.750 | 48.332 | | |
| ATOM - | 72 | С | ASP A | 11 | 41.929 | 42.813 | 47.341 | 1.00 34.03 | AAAA |
| | 73 | ō | ASP A | 11 | 41.629 | 42.652 | 46.150 | 1.00 34.80 | AAAA |
| ATOM | | | | | 41.142 | 42.417 | 48.335 | 1.00 32.34 | AAAA |
| ATOM | 74 | N | TYR A | 12 | | | | | AAAA |
| MOTA | 75 | CA | TYR A | 12 | 39.871 | 41.803 | 48.017 | 1.00 32.53 | |
| ATOM | 76 | CB | TYR A | 12 | 39.043 | 41.569 | 49.290 | 1.00 31.32 | AAAA |
| | 77 | CG | TYR A | 12 | 39.551 | 40.438 | 50.162 | 1.00 29.95 | AAAA |
| MOTA | | | | | | 40.669 | 51.469 | 1.00 28.52 | AAAA |
| ATOM | 78 | | TYR A. | 12 | 39.983 | | | | AAAA |
| ATOM | 79 | CE1 | TYR A | 12 | 40.413 | 39.614 | 52.279- | 1.00 28.03 | |
| ATOM | 80 | CD2 | TYR A | 12 | 39.568 | 39.128 | 49.688 | 1.00 28.47 | AAAA |
| | | CE2 | TYR A | 12 | 39.992 | 38.083 | 50.483 | 1.00 28.47 | AAAA |
| MOTA | 81 | _ | | | • | | 51.775 | 1.00 28.43 | - AAAA |
| ATOM | . 82 | CZ | TYR A | 12 | 40.408 | 38.330 | | | |
| ATOM | 83 | OH | TYR A | 12 | 40.786 | 37.277 | 52.569 | 1.00 29.86 | AAAA |
| ATOM | 84 | С | TYR A | 12 | 39.146 | 42.749 | 47.066 | 1.00 33.16 | . AAAA |
| | | | TYR A | 12 | 38.554 | 42.324 | 46.082 | 1.00 33.36 | AAAA |
| ATOM | 85 | 0 | | | | | 47.356 | 1.00 34.76 | AAAA |
| MOTA | 86 | N | GLY A | 13 | 39.237 | 44.041 | | | |
| ATOM | 87 | CA | GLY A | 13 | 38.594 | 45.065 | 46.546 | 1.00 36.60 | AAAA |
| | 88 | C | GLY A | 13 | 38.814 | 44.961 | 45.052 | 1.00 37.85 | AAAA |
| ATOM | | | | 13 | 38.105 | 45.591 | 44.275 | 1.00 37.40 | AAAA |
| MOTA | 89 | 0 | GLY A | | | | 44.647 | 1.00 39.55 | AAAA |
| ATOM | 90 | N | LYS A | 14 | 39.799 | 44.171 | | | |
| MOTA | 91 | CA | LYS A | 14 | 40.091 | 43.981 | 43.231 | 1.00 40.66 | AAAA |
| ATOM | 92 | CB | LYS A | 14 | 41.605 | 43.977 | 42.995 | 1.00 42.26 | AAAA |
| | | | LYS A | 14 | 42.300 | 45.309 | 43.239 | 1.00 44.54 | AAAA |
| MOTA | 93 | CG | | | | 46.445 | 42.304 | 1.00 46.32 | AAAA |
| MOTA | 94 | CD | LYS A | 14 | 41.820 | | | | AAAA |
| MOTA | 95 | CE | LYS A | 14 | 42.033 | 46.158 | 40.810 | 1.00 46.64 | |
| MOTA | 96 | NZ | LYS A | 14 | 41.133 | 45.086 | 40.256 | 1.00 47.23 | AAAA |
| | 97 | | LYS A | 14 | 39.499 | 42.675 | 42.707 | 1.00 40.35 | AAAA |
| ATOM | | C | | | | 42.377 | 41.511 | 1.00 39.97 | AAAA |
| ATOM | 98 | 0 | LYS A | 14 | 39.593 | | | | AAAA |
| MOTA | 99 | N | TYR A | 15 | 38.897 | 41.901 | 43.605 | 1.00 39.95 | |
| MOTA | 100 | CA | TYR A | 15 | . 38.300 | 40.617 | 43.245 | 1.00 40.30 | AAAA |
| | | CB | TYR A | 15 | 38.962 | 39.490 | 44.050 | 1.00 38.46 | AAAA |
| ATOM | 101 | | | | 40.472 | 39.519 | 44.021 | 1.00 37.01 | AAAA |
| ATOM | 102 | CG | TYR A | 15 | | | | 1.00 36.24 | AAAA |
| MOTA | 103 | CD1 | TYR A | 15 | 41.213 | 39.136 | 45.137 | | |
| ATOM | 104 | CE1 | TYR A | 15 | 42.604 | 39.220 | 45.144 | 1.00 35.73 | AAAA |
| | 105 | CD2 | TYR A | 15 | 41.163 | 39.976 | 42.902 | 1.00 36.84 | AAAA |
| ATOM | | | | 15 | 42.556 | 40.064 | 42.898 | 1.00 36.53 | AAAA |
| MOTA | 106 | CE2 | TYR A | | | | 44.028 | 1.00 36.24 | AAAA |
| ATOM | 107 | cz | TYR A | 15 | 43.271 | 39.689 | | | AAAA |
| MOTA | 108 | OH | TYR A | 15 | 44.648 | 39.816 | 44.042 | 1.00 36.49 | |
| | 109 | C | TYR A | 15 | 36.802 | 40.647 | 43.556 | 1.00 41.98 | AAAA |
| MOTA | | | | 15 | 36.288 | 39.786 | 44.280 | 1.00 42.59 | AAAA |
| MOTA | 110 | 0 | TYR A | | | | 43.014 | 1.00 42.81 | · AAAA |
| ATOM | 111 | N | ARG A | 16 | 36.101 | 41.638 | | | AAAA |
| ATOM | 112 | CA | ARG A | 16 | 34.670 | 41.753 | 43.257 | 1.00 43.47 | |
| | 113 | CB | ARG A | 16 | 34.205 | 43.197 | 43.111 | 1.00 45.27 | AAAA |
| MOTA | | | | 16 | 35.021 | 44.234 | 43.833 | 1.00 48.06 | AAAA |
| ATOM | 114 | CG | ARG A | | | 44.196 | 45.339 | 1.00 49.63 | AAAA |
| ATOM | 115 | CD | ARG A | 16 | 34.891 | | | 1.00 51.65 | AAAA |
| ATOM | 116 | NE | ARG A | 16 | 35.632 | 45.322 | 45.905 | | |
| | 117 | CZ | ARG A | 16 | 35.382 | 46.602 | 45.622 | 1.00 52.71 | AAAA |
| ATOM | | | ARG A | 16 | 34.406 | 46.931 | 44.781 | 1.00 53.28 | AAAA |
| ATOM | 118 | | | | | | 46.162 | 1.00 53.43 | AAAA |
| ATOM | 119 | NH2 | ARG A | 16 | 36.124 | 47.560 | | 1.00 33.45 | AAAA |
| MOTA | 120 | С | ARG A | 16 | 33.913 | 40.929 | 42.230 | 1.00 42.86 | |
| | 121 | 0 | ARG A | 16 | 34.455 | 40.541 | 41.193 | 1.00 41.83 | AAAA |
| ATOM | | | | | 32.651 | 40.668 | 42.523 | 1.00 42.42 | AAAA |
| ATOM | 122 | N | TYR A | 17 | | | 41.590 | 1.00 42.76 | AAAA |
| ATOM | 123 | CA | TYR A | 17 | 31.818 | 39.942 | | 1.00 40 10 | AAAA |
| ATOM | 124 | CB | TYR A | 17 | 30.675 | 39.254 | 42.333 | 1.00 40.11 | |
| | | | TYR A | 17 | 31.097 | 38.061 | 43.180 | 1.00 38.35 | AAAA |
| ATOM | 125 | CG | | | 32.169 | 38.148 | 44.071 | 1.00 36.15 | AAAA |
| ATOM | 126 | CD1 | TYR A | 17 | | | | 1.00 34.76 | AAAA |
| ATOM | 127 | CE1 | TYR A | 17 | 32.519 | 37.069 | 44.874 | 1.00 31.70 | AAAA |
| | 128 | CD2 | TYR A | 17 | 30.386 | 36.855 | 43.116 | 1.00 36.40 | |
| ATOM | | | | 17 | 30.726 | 35.776 | 43.912 | 1.00 35.31 | AAAA |
| MOTA | 129 | CE2 | TYR A | | | 35.887 | 44.790 | 1.00 35.00 | AAAA |
| MOTA | 130 | CZ | TYR A | 17 | 31.792 | | | 1.00 33.29 | AAAA |
| ATOM | 131 | OH | TYR A | 17 | 32.115 | 34.814 | 45.584 | 1.00 33.29 | |
| | 132 | C | TYR A | 17 | 31.296 | 41.000 | 40.613 | 1.00 44.43 | AAAA |
| MOTA | 134 | _ | | | 32.230 | | - | | • |
| - | | | | | | | | | |

| MOTA | 13: | 3 0 | TY | RA | 17 | 31.346 | 42.194 | 40.905 | 1.00 44.68 | AAAA |
|--------------|-----|------|---------|-----|----------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 134 | 1 N | PR | O A | 18 | 30.799 | | | | AAAA |
| ATOM | 13 | 5 CI |) PR | O A | 18 | 30.707 | | | | AAAA |
| MOTA | 136 | 5 C2 | A PR | O A | 18 | 30.268 | | | | AAAA |
| ATOM | 137 | 7 CI | 3 PR | O A | | 29.854 | | | | AAAA |
| ATOM | 138 | 3 CC | PR | O A | 18 | 30.876 | | | | AAAA |
| ATOM | 139 |) c | | O A | | 29.129 | | | | , m |
| MOTA | 140 | | | OA | | 28.298 | | | | AAAA |
| ATOM | 141 | | | SA | | 29.114 | | | | AAAA |
| ATOM | 142 | | | SA | | 28.125 | | | | AAAA |
| ATOM | 143 | | | SA | | 27.876 | | | | AAAA |
| ATOM | 144 | | | SA | | 29.120 | | | | AAAA |
| ATOM | 145 | | | SA | | 28.747 | | | 1.00 57.78 | AAAA |
| ATOM | 146 | | | S A | | 29.978 | | 34.288 | | AAAA |
| ATOM | 147 | | | 5 A | | 29.616 | | 32.932 | | AAAA |
| ATOM | 148 | | LYS | | | 26.764 | | | 1.00 61.03 | AAAA |
| ATOM | 149 | | LYS | | 19 | 26.281 | | 39.012 | 1.00 51.53 | AAAA |
| ATOM | 150 | | ASN | | 20 | 26.146 | 44.556 | 40.071 | 1.00 51.54 | AAAA |
| ATOM | 151 | | | | 20 | • | 43.314 | 38.203 | 1.00 50.13 | AAAA |
| ATOM | 152 | | | | 20 | 24.831 | 42.750 | 38.482 | 1.00 48.44 | AAAA |
| ATOM | 153 | | | | 20 | 24.336 | 42.061 | | 1.00 49.67 | AAAA |
| ATOM | 154 | | 1 ASN | | 20 | 25.389 | 41.132 | 36.613 | 1.00 51.61 | AAAA |
| ATOM | 155 | | 2 ASN | | 20 | 25.677 | 40.064 | 37.154 | 1.00 51.70 | AAAA |
| ATOM | 156 | C | 2 ASN | | 20 | 25.998 | 41.562 | 35.509 | 1.00 53.00 | аааа |
| ATOM | 157 | ō | ASN | | 20 | 24.789 23.764 | 41.765 | 39.649 | 1.00 45.57 | AAAA |
| ATOM | 158 | N | HIS | | 21 | | 41.127 | 39.877 | 1.00 44.67 | AAAA |
| ATOM | 159 | CA | HIS | | 21 | 25.883 | 41.662 | 40.398 | 1.00 42.71 | AAAA |
| MOTA | 160 | CB | HIS | | 21 | 25.958 | 40.709 | 41.506 | 1.00 40.69 | AAAA |
| ATOM | 161 | CG | HIS | | 21 | 27.216 27.186 | 39.857 | 41.353 | 1.00 40.16 | AAAA |
| MOTA | 162 | | 2 HIS | | 21 | 27.186 | 38.587 | 42.140 | 1.00 39.93 | AAAA |
| ATOM | 163 | | l HIS | | 21 | 26.951 | 38.353 | 43.467 | 1.00 39.27 | AAAA |
| ATOM | 164 | | l HIS | | 21 | 26.931 | 37.359 | 41.557 | 1.00 39.47 | AAAA |
| ATOM | 165 | | HIS | | 21 | 27.174 | 36.425 | 42.493 | 1.00 39.36 | AAAA |
| MOTA | 166 | C | HIS | | 21 | 25.974 | 37.003 41.349 | 43.660 | 1.00 39.44 | AAAA |
| MOTA | 167 | õ | HIS | | 21 | 26.660 | 41.349 | 42.892 | 1.00 38.93 | AAAA |
| ATOM | 168 | N | PRO | | 22 | 25.229 | 40.778 | 43.116 | 1.00 38.78 | AAAA |
| ATOM | 169 | CD | PRO | | 22 | 24.371 | 39.579 | 43.853 | 1.00 37.11 | AAAA |
| ATOM | 170 | CA | PRO | | 22 | 25.224 | 41.361 | 43.814 45.199 | 1.00 36.09 | AAAA |
| ATOM | 171 | CB | PRO | | 22 | 24.473 | 40.306 | 46.012 | 1.00 35.81 | AAAA |
| MOTA | 172 | CG | PRO | | 22 | 23.464 | 39.810 | 45.003 | 1.00 36.04 | AAAA |
| ATOM | 173 | c | PRO | | 22 | 26.638 | 41.637 | 45.751 | 1.00 36.19 1.00 34.39 | AAAA |
| ATOM | 174 | ŏ | PRO | | 22 | 26.867 | 42.653 | 46.417 | | AAAA |
| ATOM | 175 | N | LEU | | 23 | 27.572 | 40.731 | 45.451 | 1.00 34.09 1.00 31.98 | AAAA |
| ATOM | 176 | CA | LEU | | 23 | 28.954 | 40.827 | 45.900 | 1.00 31.98 | AAAA |
| ATOM | 177 | CB | LEU | | 23 | 29.564 | 39.432 | 46.014 | 1.00 27.88 | AAAA |
| ATOM | 178 | CG | LEU | | 23 | 28.896 | 38.528 | 47.048 | 1.00 27.33 | AAAA |
| ATOM | 179 | | LEU | | 23 | 29.656 | 37.217 | 47.149 | 1.00 26.64 | AAAA |
| ATOM | 180 | | LEU | | 23 | 28.879 | 39.212 | 48.399 | 1.00 26.75 | 1AAA |
| ATOM | 181 | С | LEU | | 23 | 29.838 | 41.709 | 45.018 | 1.00 29.20 | AAAA |
| ATOM | 182 | 0 | LEU | | 23 | 31.057 | 41.606 | 45.028 | 1.00 28.38 | AAAA |
| MOTA | 183 | N | LYS | | 24 | 29.204 | | 44.259 | 1.00 29.27 | AAAA |
| ATOM | 184 | CA | LYS | A | 24 | 29.903 | 43.512 | | . 1.00 29.30 | AAAA |
| ATOM | 185 | CB | LYS | | 24 | 28.881 | 44.091 | 42.405 | 1.00 29.75 | AAAA AAAA |
| ATOM | 186 | CG | LYS | | 24 | 29.328 | 45.265 | 41.601 | 1.00 32.55 | |
| ATOM | 187 | CD | LYS | | 24 | 28.537 | 46.526 | 41.994 | 1.00 34.37 | AAAA |
| ATOM | 188 | CE | LYS | | 24 | 27.025 | 46.337 | 41.835 | 1.00 34.32 | AAAA |
| MOTA | 189 | NZ | LYS | | 24 | 26.221 | 47.542 | 42.208 | 1.00 34.32 | AAAA |
| ATOM | 190 | C | LYS | | 24 | 30.580 | 44.620 | 44.224 | 1.00 34.37 | AAAA |
| ATOM | 191 | ō | LYS . | | 24 | 31.617 | 45.162 | 44.224 | | AAAA |
| ATOM | 192 | Ŋ | ILE . | | 25 | 29.990 | 44.919 | 45.377 | 1.00 27.93 | AAAA |
| ATOM | 193 | CA | ILE . | | 25 | 30.468 | 44.919 | 45.377 | 1.06 27.07 | AAAA |
| ATOM | 194 | CB | ILE . | | 25 | 29.425 | 45.945 | | 1.00 25.82 | AAAA . |
| | 195 | | ILE A | | 25 25 | 28.190 | | 47.364 | 1.00 25.37 | AAAA |
| MOTA MOTA | 196 | | ILE A | | 25 25 | 29.142 | 46.846 44.979 | 46.737 | 1.00 25.71 | AAAA |
| ATOM | 197 | | ILE A | | 25 25 | 28.318 | 44.979 | 48.157 49.413 | 1.00 25.26 1.00 25.17 | AAAA |
| ATOM | 198 | CDI | ILE A | | 25 25 | 31.700 | | 47.095 | | AAAA |
| ATOM. | 100 | ٠. | 1 JUE 1 | ra. | | 31.700 | 45.550 | 91.UJO - | 1.00 25.28 | AAAA |

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| ATOM | 199 | 0 | ILE A | 25 | 32.037 | 44.379 | 47.183 | 1.00 24.48 | AAAA · |
|--------|-----|-----|-------|------|--------|--------|--------------------|------------|--------|
| ATOM | 200 | Ŋ | PRO A | | 32.375 | 46.547 | 47.714 | 1.00 24.98 | AAAA |
| | 201 | CD | PRO A | | 32.062 | 47.980 | 47.638 | 1.00 24.98 | AAAA |
| ATOM | | | | | 33.570 | 46.367 | 48.543 | 1.00 24.44 | AAAA |
| ATOM | 202 | CA | PRO A | | | 47.792 | 48.701 | 1.00 24.75 | AAAA |
| ATOM | 203 | CB | PRO A | _ | 34.094 | | | 1.00 25.51 | |
| MOTA | 204 | CG | PRO A | . 26 | 33.435 | 48.546 | 47.538 | | AAAA |
| ATOM | 205 | С | PRO A | . 26 | 33.021 | 45.838 | 49.862 | 1.00 23.42 | AAAA |
| ATOM | 206 | ၁ | PRO A | 26 | 31.930 | 46.233 | 50.272 | 1.00 22.12 | AAAA |
| ATOM | 207 | N | ARG A | 27 | 33.754 | 44.960 | 50.532 | 1.00 23.06 | AAAA |
| | 208 | CA | ARG A | | 33.244 | 44.421 | 51.776 | 1.00 23.04 | AAAA |
| ATOM | _ | CB | ARG A | | 32.633 | 43.043 | 51.492 | 1.00 22.20 | AAAA |
| ATOM | 209 | | | | 31.463 | 43.152 | 50.503 | 1.00 19.84 | AAAA |
| ATOM | 210 | CG | ARG A | | | | 50.160 | 1.00 18.64 | AAAA |
| MOTA | 211 | CD | ARG A | | 30.762 | 41.844 | | | AAAA |
| ATOM | 212 | NE | ARG A | | 30.181 | 41.168 | 51.315 | 1.00 16.51 | |
| ATOM | 213 | CZ | ARG A | . 27 | 30.774 | 40.188 | 51.982 | 1.00 16.57 | AAAA |
| ATOM | 214 | NH1 | ARG A | . 27 | 31.969 | 39.763 | 51.605 | 1.00 17.50 | AAAA |
| ATOM | 215 | | ARG A | 27 | 30.185 | 39.643 | 53.038 | 1.00 16.45 | AAAA |
| | 216 | C | ARG A | | 34.265 | 44.381 | 52.905 | 1.00 23.62 | AAAA |
| ATOM | | | ARG A | | 34.107 | 45.077 | 53.919 | 1.00 23.69 | AAAA |
| MOTA | 217 | 0 | | | 35.305 | 43.570 | 52.736 | 1.00 24.25 | AAAA |
| · ATOM | 218 | N | VAL A | | | 43.466 | 53.737 | 1.00 23.36 | AAAA |
| ATOM | 219 | CA | VAL A | | 36.355 | | | 1.00 22.75 | AAAA |
| MOTA | 220 | CB | VAL A | | 37.022 | 42.062 | 53.671 | | |
| MOTA | 221 | CG1 | VAL A | . 28 | 38.292 | 42.031 | 54.475 | 1.00 22.95 | AAAA |
| ATOM | 222 | CG2 | VAL A | . 28 | 36.061 | 41.011 | 54.249 | 1.00 22.20 | AAAA |
| ATOM | 223 | С | VAL A | 28 | 37.363 | 44.609 | 53.511 | 1.00 23.70 | aaaa |
| ATOM | 224 | 0 | VAL A | 28 | 37.943 | 45.156 | 54.455 | 1.00 22.62 | aaaa |
| ATOM | 225 | N | SER A | | 37.538 | 44.989 | 52.253 | 1.00 24.27 | አሕአA |
| | 226 | CA | SER A | | 38.444 | 46.082 | 51.910 | 1.00 26.03 | aaaa |
| ATOM | | CB | SER A | | 38.632 | 46.178 | 50.381 | 1.00 25.95 | AAAA |
| MOTA | 227 | | | | 37.395 | 46.417 | 49.716 | 1.00 27.57 | AAAA |
| MOTA | 228 | og | SER A | | 37.793 | 47.354 | 52.440 | 1.00 25.52 | AAAA |
| MOTA | 229 | C | SER A | | | | 52.828 | 1.00 25.49 | AAAA |
| ATOM | 230 | 0 | SER A | | 38.463 | 48.311 | | | AAAA |
| ATOM | 231 | N | LEU A | . 30 | 36.468 | 47.342 | 52.448 | 1.00 26.09 | |
| MOTA | 232 | CA | LEU A | . 30 | 35.692 | 48.471 | 52.926 | 1.00 26.39 | AAAA |
| ATOM | 233 | CB | LEU A | . 30 | 34.262 | 48.365 | 52.393 | 1.00 25.89 | AAAA |
| ATOM | 234 | CG | LEU A | 30 | 33.265 | 49.470 | 52.755 | 1.00 27.15 | AAAA |
| ATOM | 235 | | LEU A | 30 | 32.486 | 49.101 | 53.99 9 | 1.00 26.34 | AAAA |
| | 236 | | LEU A | | 34.015 | 50.813 | 52.897 | 1.00 25.81 | AAAA |
| MOTA | 237 | c | LEU A | | 35.713 | 48.534 | 54.453 | 1.00 26.26 | AAAA |
| MOTA | | | LEU A | | 35.731 | 49.612 | 55.037 | 1.00 27.50 | AAAA |
| ATOM | 238 | 0 | | | 35.730 | 47.379 | 55.097 | 1.00 25.57 | AAAA |
| MOTA | 239 | N | LEU A | | 35.776 | 47.343 | 56.545 | 1.00 26.87 | AAAA |
| MOTA | 240 | CA | LEU A | | | 45.900 | 57.029 | 1.00 27.28 | AAAA |
| MOTA | 241 | CB | LEU A | | 35.752 | | 58.383 | 1.00 27.87 | AAAA |
| MOTA | 242 | CG | LEU A | | 35.135 | 45.563 | | 1.00 27.01 | AAAA |
| MOTA | 243 | | LEU A | | 35.855 | 44.313 | 58.906 | | |
| ATOM | 244 | CD2 | LEU A | 31 | 35 261 | 46.706 | 59.372 | 1.00 26.32 | AAAA |
| MOTA | 245 | С | LEU A | 31 | 31.087 | 48.003 | 57.012 | 1.00 28.08 | AAAA |
| MOTA | 246 | 0 | LEU A | 31 | 37 094 | 48.854 | 57.901 | 1.00 27.42 | AAAA |
| ATOM | 247 | N | LEU A | 32 | 38.197 | 47.584 | 56.409 | 1.00 29.52 | AAAA |
| | 248 | CA | LEU A | | 39.508 | 48.121 | 56.750 | 1.00 30.96 | AAAA |
| MOTA | | | LEU A | | 40.607 | 47.394 | 55.950 | 1.00 31.58 | aaaa |
| ATOM | 249 | CB | | | 40.792 | 45.904 | 56.293 | 1.00 31.63 | AAAA |
| ATOM | 250 | CG | LEU A | | | 45.246 | 55.380 | 1.00 31.31 | AAAA |
| ATOM | 251 | | LEU A | | 41.810 | | 57.743 | 1.00 32.23 | AAAA |
| ATOM | 252 | CD2 | LEU A | | 41.232 | 45.780 | | 1.00 32.23 | AAAA |
| ATOM | 253 | С | LEU A | | 39.599 | 49.635 | 56.543 | | |
| ATOM | 254 | 0 | LEU A | 32 | 40.081 | 50.345 | 57.416 | 1.00 31.70 | AAAA |
| ATOM | 255 | N | ARG A | 33 | 39.140 | 50.129 | 55.398 | 1.00 32.72 | AAAA |
| ATOM | 256 | CA | ARG A | | 39.178 | 51.564 | 55.141 | 1.00 33.91 | AAAA |
| | 257 | CB | ARG A | | 38.643 | 51.903 | 53.743 | 1.00 35.10 | AAAA |
| ATOM | | | ARG A | | 39.627 | 51.609 | 52.621 | 1.00 37.84 | AAAA |
| ATOM | 258 | CG | | | 39.310 | 52.412 | 51.374 | 1.00 39.33 | AAAA |
| ATOM | 259 | CD | ARG A | | 38.255 | 51.806 | 50.580 | 1.00 42.51 | AAAA |
| ATOM | 260 | NE | ARG A | | | 52.395 | 49.541 | 1.00 44.22 | AAAA |
| MOTA | 261 | CZ | ARG A | | 37.662 | | 49.163 | 1.00 44.61 | AAAA |
| ATOM | 262 | NHl | ARG A | 33 | 38.016 | 53.617 | 48.861 | 1.00 45.23 | AAAA |
| ATOM | 263 | NH2 | ARG A | | 36.723 | 51.752 | | | |
| ATCM | 264 | С | ARG A | 33 | 38.352 | 52.305 | 56.168 | 1.00 33.48 | AAAA |
| | | | | | | | | | - |

| ATOM | 265 | 0 | ARG A | A 33 | 38.713 | 53.390 | · 56.592 | 1.00 33.61 | AAAA |
|-------|------|-----|---------|------|----------|--------|----------|------------|------|
| MOTA | 266 | · N | PHE | A 34 | 37.247 | | 56.562 | 1.00 33.78 | |
| | | | | | | | | | AAAA |
| MOTA | 267 | CA | PHE A | | 36.292 | 52.233 | 57.517 | 1.00 33.79 | AAAA |
| ATOM | 268 | CB | PHE A | A 34 | 35.065 | 51.310 | 57.573 | 1.00 33.88 | AAAA |
| ATOM | 269 | CG | PHE A | A 34 | 33.925 | 51.840 | 58.405 | 1.00 3316 | |
| | 270 | | | | 33.108 | | | | AAAA |
| MOTA | | | L PHE 2 | | | 52.856 | 57.925 | 1.00 32.77 | AAAA |
| ATOM | 271 | CD | PHE ? | 34 | 33.668 | 51.315 | 59.672 | 1.00 33.05 | AAAA |
| ATOM | 272 | CE. | PHE A | 34 | 32.044 | 53.343 | 58.695 | | |
| | | | | | | | | 1.00 32.86 | AAAA |
| ATOM | 273 | | PHE 2 | A 34 | 32.607 | 51.797 | 60.454 | 1.00 33.07 | AAAA |
| MOTA | 274 | CZ | PHE A | A 34 | 31.794 | 52.809 | 59.966 | 1.00 32.58 | AAAA |
| MOTA | 275 | С | PHE A | 34 | - 36.881 | 52.414 | 58.918 | 1.00 34.01 | |
| | | | | | | | | | AAAA |
| MOTA | 276 | O, | PHE ? | | 36.903 | 53.524 | 59.455 | 1.00 33.49 | AAAA |
| MOTA | 277 | N | LYS A | 35 | 37.350 | 51.324 | 59.516 | 1.00 34.00 | AAAA |
| MOTA | 278 | CA | LYS A | 35 | 37.928 | 51.401 | 60.843 | 1.00 33.90 | |
| ATOM | 279 | CB | LYS A | | | | | | AAAA |
| | | | | | 38.230 | 50.010 | 61.362 | 1.00 34.07 | AAAA |
| ATOM | 280 | CG | LYS A | 35 | 37.000 | 49.190 | 61.662 | 1.00 33.94 | AAAA |
| ATOM | 281 | CD | LYS A | 35 | 37.414 | 47.810 | 62.106 | 1.00 35.31 | AAAA |
| ATOM | 282 | CE | LYS A | | | | | | |
| | | | | | . 38.062 | 47.072 | 60.948 | 1.00 35.91 | AAAA |
| MOTA | 283 | NZ | LYS A | | 39.058 | 47.928 | 60.236 | 1.00 36.19 | AAAA |
| ATOM | 284 | С | LYS A | 35 | 39.185 | 52.255 | 60.881 | 1.00 34.19 | AAAA |
| MOTA | 285 | ο. | LYS A | | 39.554 | 52.775 | 61.929 | | |
| | • | | | | | | | 1.00 34.32 | AAAA |
| ATOM | 286 | N | ASP A | | 39.853 | 52.384 | 59.745 | 1.00 33.99 | AAAA |
| ATOM | 287 | ÇA | ASP A | . 36 | 41.034 | 53.216 | 59.680 | 1.00 35.17 | AAAA |
| ATOM | 288 | CB | ASP A | 36 | 41.812 | 52.943 | 58.388 | 1.00.37.40 | |
| ATOM | 289 | ÇG | ASP A | | | | | | AAAA |
| 6.1 | | | | | 42.964 | 53.908 | 58.186 | 1.00 38.64 | AAAA |
| MOTA | 290 | OD1 | ASP A | . 36 | 43.648 | 54.218 | 59.184 | 1.00 40.02 | AAAA |
| ATOM | 291 | OD2 | ASP A | 36 | 43.201 | 54.341 | 57.035 | 1.00 38.74 | AAAA |
| ATOM | 292 | С | ASP A | 36 | 40.568 | 54.670 | 59.724 | 1.00 35.85 | |
| | | | | | | | | | AAAA |
| ATOM | 293 | 0 | ASP A | | 41.231 | 55.527 | 60.306 | 1.00 36.88 | AAAA |
| ATOM- | 294 | N | ALA A | . 37 | 39.420≀ | 54.940 | 59.111 | 1.00 34.96 | AAAA |
| MOTA | 295 | CA | ALA A | . 37 | 38.851 | 56.280 | 59.108 | 1.00 34.47 | AAAA |
| ATOM | 296 | CB | ALA A | | 37.751 | 56.373 | | | |
| | | | _ | | | _ | 58.067 | 1.00 33.80 | AAAA |
| ATOM | 297 | С | ALA A | | 38.291 | 56.617 | 60.499 | 1.00 34.66 | AAAA |
| MOTA | 298 | Q | ALA A | 37 | 38.268 | 57.779 | 60.899 | 1.00 34.55 | AAAA |
| MOTA | 299 | N | MET A | 3'8 | 37.830 | 55.600 | 61.226 | 1.00 34.24 | AAAA |
| ATOM | 300 | CA | MET A | | | | | | |
| | | | | | 37.287 | 55.794 | 62.572 | 1.00 33.07 | AAAA |
| ATOM | 301 | CB | MET A | 38 | 36.289 | 54.687 | 62.917 | 1.00 32.82 | AAAA |
| MOTA | 302 | CG | MET A | 38 | 35.084 | 54.559 | 61.996 | 1.00 32.72 | AAAA |
| ATOM | 303 | SD | MET A | 38 | 33.980 | 55.948 | 62.101 | 1.00 33.65 | AAAA |
| | 304 | CE | | | | | | | |
| ATOM | | | MET A | 38 | 33.550 | 55.878 | 63.849 | 1.00 33.77 | AAAA |
| ATOM | 305 | C | MET A | 38 | 38.430 | 55.724 | 63.583 | 1.00 33.12 | AAAA |
| ATOM | 306 | 0 | MET A | 38 | 38.226 | 55.930 | 64.777 | 1.00 32.82 | AAAA |
| MOTA | 307 | N | ASN A | 39 | 39.628 | 55.428 | 63.090 | 1.00 32.64 | |
| | | | | | | | | | AAAA |
| ATOM | 308 | CA | ASN A | 39 | 40.805 | 55.266 | 63.935 | 1.00 32.38 | AAAA |
| ATOM | 309 | CB | ASN A | 39 | 41.200 | 56.600 | 64.589 | 1.00 32.93 | AAAA |
| ATOM | 310 | CG | ASN A | 39 | 41.393 | 57.736 | 63.571 | 1.00 34.40 | AAAA |
| ATOM | 311 | | ASN A | 39 | 42.180 | 57.624 | 62.630 | 1.00 34.98 | |
| | | | | | | | | | AAAA |
| ATOM | 312 | | ASN A | 39 | 40.677 | 58.838 | 63.772 | 1.00 33.52 | AAAA |
| ATOM | 313 | С | ASN A | 39 | 40.483 | 54.212 | 65.009 | 1.00 31.69 | AAAA |
| ATOM | 314 | 0 | ASN A | 39 | ·40.565 | 54.490 | 66.205 | 1.00 31.12 | AAAA |
| ATOM | 315 | | LEU A | 40 | | | | | |
| | | N | | | 40.095 | 53.010 | 64.570 | 1.00 31.76 | AAAA |
| ATOM | 316 | CA | LEU A | 40 | 39.750 | 51.898 | 65.474 | 1.00 32.48 | AAAA |
| ATOM | 317 | CB | LEU A | 40 | 38.259 | 51.559 | 65.386 | 1.00 32.55 | AAAA |
| | .318 | CG | LEU A | 40 | 37.231 | 52.581 | | 1.00 32.84 | |
| | | | | | | | | | AAAA |
| ATOM | 319 | | LEU A | 40 | 35.837 | 52.089 | 65.554 | 1.00 33.79 | AAAA |
| MOTA | 320 | CD2 | LEU A | 40 | 37.372 | 52.798 | 67.376 | 1.00 32.45 | AAAA |
| ATOM | 321 | С | LEU A | 40 | 40.555 | 50.628 | 65.187 | 1.00 32.92 | AAAA |
| ATOM | 322 | | LEU A | 40 | | | | | |
| | | 0 | | | 40.196 | 49.530 | 65.618 | 1.00 31.64 | AAAA |
| ATOM | 323 | N | ILE A | 41 | 41.652 | 50.794 | 64.464 | 1.00 34.12 | aaaa |
| ATOM | 324 | CA | ILE A | 41 | 42.508 | 49.680 | 64.116 | 1.00 36.07 | AAAA |
| ATOM | 325 | СВ | ILE A | 41 | 42.017 | 48.991 | 62.811 | 1.00 35.51 | |
| | | | | | | | | | AAAA |
| ATOM | 326 | | ILE A | 41 | 42.070 | 49.952 | 61.636 | 1.00 33.37 | AAAA |
| ATOM | 327 | CG1 | ILE A | 41 | 42.898 | 47.790 | 62.480 | 1.00 35.97 | AAAA |
| ATOM | 328 | | ILE A | 41 | 42.854 | 46.701 | 63.500 | 1.00 37.19 | AAAA |
| | | | | | | | | 1.00 38.85 | |
| ATOM | 329 | С | ILE A | 41 | 43.921 | 50.226 | 63.916 | | AAAA |
| MOTA | 330 | 0 | ILE A | 41 | 44.106 | 51.346 | 63.413 | 1.00 38.98 | AAAA |

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| ATOM . | 331 | N | ASP | Α | 42 | 44.914 | 49.446 | 64.329 | 1.00 40.61 | AAAA |
|--------------|------------|---------|-------|----|----------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 332 | CA | AŞP | Α | 42 | 46.309 | 49.843 | 64.181 | 1.00 42.57 | AAAA |
| ATOM | 333 | CB | ASP | Α | 42 | 46.973 | 50.021 | 65.553 | 1.00 42.42 | AAAA |
| ATOM | 334 | CG | ASP | A | 42 | 46.316 | 51.110 | 66.381 | 1.00 42.27 | AAAA |
| MOTA | 335 | OD1 | ASP | A | 42 | 46.227 | 52.250 | 65.883 | 1.00 41.20 | AAAA |
| ATOM_ | 336 | OD2 | ASP | A | 42 | 45.891 | 50.833 | 67.526 | 1.00 43.36 | AAAA |
| ATOM | 337 | С | ASP | | 42 | 47.011 | 48.752 | 63.392 | 1.00 44.05 | AAAA |
| MOTA | 338 | 0 | ASP | Α | 42 | 46.525 | 47.620 | 63.333 | 1.00 44.88 | AAAA |
| ATOM | 339 | N | GLU | | 43 | 48.147 | 49.090 | 62.789 | 1.00 45.10 | AAAA |
| ATOM | 340 | CA | _GLU | Α | 43 | 48.905 | 48.141 | 61.980 | 1.00 46.11 | AAAA |
| ATOM | 341 | CB | GLU | Α | 43 | 50.172 | 48.796 | 61.454 | 1.00 46.89 | AAAA |
| MOTA | 342 | CG | GLU | A. | 43 | 49.924 | 50.057 | 60.668 | 1.00 49.30 | AAAA |
| ATOM | 343 | CD | GLU | A | 43 | · 51.187 | 50.580 | 60.028 | 1.00 49.67 | AAAA |
| ATOM | 344 | OE1 | GLU | Α | 43 | 51.760 | 49.839 | 59.201 | 1.00 50.60 | AAAA |
| ATOM | 345 | OE2 | GLU | А | 43 | 51.601 | 51.714 | 60.349 | 1.00 49.60 | AAAA |
| MOTA | 346 | С | GLU | Α | 43 | 49.290 | 46.859 | 62.701 | 1.00 46.27 | - AAAA |
| ATOM | 347 | 0 | GLU | A | 43 | 49.214 | 45.773 | 62.131 | 1.00 46.00 | AAAA |
| ATOM | 348 | N | LYS | Α | 44 | 49.708 | 46.986 | 63.954 | 1.00 46.52 | AAAA |
| MOTA | 349 | CA | LYS | Α | 44 | 50.135 | 45.832 | 64.730 | 1.00 46.31 | |
| ATOM | 350 | CB | LYS | | 44 | 50.762 | 46.306 | 66.048 | 1.00 48.16 | |
| MOTA | 351 | CG | LYS | Α | 44 | 51.977 | 47.215 | 65.799 | 1.00 51.59 | AAAA |
| MOTA | 352 | CD | LYS | Α | 44 | 52.641 | 47.734 | 67.071 | 1.00 52.87 | - |
| MOTA | 353 | CE | LYS | | 44 | 53.851 | 48.601 | 66.727 | 1.00 53.34 | |
| ATOM | 354 | NZ | LYS | | 44 | 54.615 | 49.033 | 67.936 | 1.00 53.45 | |
| MOTA | 355 | С | LYS | | 44 | 49.029 | 44.828 | 64.996 | 1.00 44.74 | |
| ATOM | 356 | 0 | LYS | | 44 | 49.296 | 43.735 | 65.480 | 1.00 45.35 | |
| MOTA | 357 | N | GLU | | 45 | 47.793 | 45.190 | 64.659 | 1.00 42.49 | |
| MOTA | 358 | CA | GLU | | 45 | 46.638 | 44.320 | 64.894 | 1.00 40.54 | |
| ATOM | 359 | CB | GLU | | 45 | 45.493 | 45.125 | 65.517 | 1.00 40.55 | |
| ATOM | 360 | CG | GLU | | 45 | 45.788 | 45.731 | 66.882 | 1.00 38.87 | |
| MOTA | 361 | CD | GLU | | 45 | 44.663 | 46.618 | 67.360 | 1.00 37.57 | |
| MOTA | 362 | | GLU | | 45 | 44.383 | 47.631 | 66.693 | 1.00 36.29 | |
| ATOM | 363 | | GLU | | 45 | 44.056 | 46.300 | 68.399 | 1.00 38.44 | |
| ATOM | 364 | C | GLU | | 45 | 46.126 | 43.648 42.737 | 63.630 63.681 | 1.00 39.15 1.00 39.29 | |
| ATOM | 365 366 | 0 | GLU | | 45 46 | 45.301 46.619 | 44.115 | 62.497 | 1.00 37.62 | |
| MOTA | 367 | N CA | LEU | | 46 | 46.219 | 43.589 | 61.211 | 1.00 37.82 | |
| ATOM | 368 | CB | LEU | | 46 | 46.125 | 44.750 | 60.229 | 1.00 35.88 | |
| MOTA MOTA | 369 | CG | LEU | | 46 | 45.608 | 44.550 | 58.817 | 1.00 36.50 | |
| ATOM | 370 | | LEU | | 46 | 44.182 | 44.021 | 58.843 | 1.00 36.66 | |
| ATOM | 371 | | LEU | | 46 | 45.646 | 45.893 | 58.113 | 1.00 35.85 | |
| ATOM | 372 | c | LEU | | 46 | 47.211 | 42.542 | 60.714 | 1.00 34.97 | |
| ATOM | 373 | ō | LEU | | 46 | 48.424 | 42.670 | 60.900 | 1.00 35.72 | |
| ATOM | 374 | N | ILE | | 47 | 46.680 | 41.484 | 60.118 | 1.00 33.25 | |
| ATOM | 375 | CA | ILE | | 47 | 47.497 | 40.411 | 59.560 | 1.00 30.92 | |
| ATOM | 376 | CB | ILE | | 47 | 47.144 | 39.024 | 60.167 | 1.00 31.22 | |
| ATOM | 377 | CG2 | ILE | | 47 | 48.093 | 37.97Ċ | 59.640 | 1.00 28.55 | AAAA |
| ATOM | 378 | CG1 | ILE | A | 47 | 47.220 | 39.063 | 61.694 | 1.00 32.04 | AAAA |
| ATOM | 379 | CD1 | ILE . | | 47 | 48.596 | 39.241 | 62.242 | 1.00 34.13 | AAAA |
| MOTA | 380 | С | ILE . | A | 47 | 47.138 | 40.381 | 58.076 | 1.00 29.70 | AAAA |
| MOTA | 381 | 0 | ILE . | A | 47 | 45.956 | 40.373 | 57.714 | 1.00 28.42 | |
| ATOM | 382 | N | LYS . | A | 48 | 48.150 | 40.380 | 57.221 | 1.00 28.78 | AAAA |
| ATOM | 383 | CA | LYS . | A | 48 | 47.920 | 40.349 | 55.784 | 1.00 28.42 | |
| ATOM | 384 | CB | LYS . | A | 48 | 49.203 | 40.727 | 55.055 | 1.00 27.53 | AAAA |
| MOTA | 385 | CG | LYS . | | 48 | 49.116 | 40.695 | 53.556 | 1.00 28.97 | AAAA |
| MOTA | 386 | CD | LYS . | A | 48 | 50.464 | 41.104 | 52.941 | 1.00 29.67 | AAAA |
| ATOM | 387 | CE | LYS . | A | 48 | 50.493 | 40.893 | 51.432 | 1.00 29.41 | |
| ATOM | 388 | NZ | LYS 2 | | 48 | 49.409 | 41.645 | 50.764 | 1.00 29.68 | |
| ATOM | 389 | C | LYS 2 | | 48 | 47.449 | 38.950 | 55.375 | 1.00 27.81 | |
| ATOM | 390 | 0 | LYS | À | 48 | 48.024 | 37.938 | 55.787 | 1.00 27.96 | |
| ATOM | 391 | И | SER A | | 49 | 46.385 | 38.892 | 54.581 | 1.00 26.82 | |
| ATOM | 392 | CA | SER . | | 49 | 45.854 | 37.611 | 54.141 | 1.00 26.41 | |
| ATOM | 393 | CB | SER | | 49 | 44.514 | 37.795 | 53.420 | 1.00 25.40 | |
| ROTE | 394 | OG | SER | | | 43.541 | 38.349 | 54.276 | 1.00 25.58 | |
| ATOM | 395 | С | SER | | 49 | 46.814 | 36.891 | 53.207 | 1.00 26.03 | |
| ATOM | 396 | 0 | SER A | A | 49 | 47.462 | 37.513 | 52.373 | 1.00 26.98 | AAAA |
| - | | _ | | | | | | | | |

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Figure 19-7

| ATOM | 397 | 7 N | AR | G A | 50 | 46.910 | 35.576 | 53.354 | 1.00 25.51 | AAAA |
|--------------|------------|------------|-------|------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 398 | C.P | A AR | G A | 50 | 47.755 | 34.794 | 52.474 | 1.00 25.45 | AAAA |
| ATOM | 399 | | AR | G A | 50 | 48.807 | 33.985 | 53.252 | 1.00 25.85 | AAAA |
| MOTA | 400 | | AR | G A | 50 | 48.229 | 32.819 | 54.009 | 1.00 27.16 | AAAA |
| MOTA | 401 | | | G A | | 49.280 | 31.995 | | 1.00 27.57 | AAAA |
| MOTA | 402 | | | G A | | 48.673 | 30.896 | 55.482 | 1.00 27.90 | AAAA |
| MOTA | 403 | | | G A | | 48.106 | 29.820 | 54.946 | 1.00 28.34 | AAAA |
| MOTA | 404 | | II AR | | | 48.055 | 29.672 | | 1.00 28.19 | AAAA |
| ATOM | 405 | | | G A | | 47.592 | 28.884 | 55.735 | 1.00 28.62 | AAAA |
| ATOM | 406 | | | G A | | 46.806 | 33.834 | 51.762 | 1.00 24.91 | AAAA |
| ATOM | 407 | | | G A | | 45.740 | 33.510 | 52.283 | 1.00 23.57 | AAAA |
| MOTA | 408 | | | O A | | 47.172 | 33.392 | 50.549 | 1.00 24.28 | AAAA |
| MOTA MOTA | 409 | | | 0 A | | 48.361 | 33.761 | 49.770 | 1.00 24.13 | AAAA . |
| ATOM | 410 411 | | | A 0 A 0 | | 46.355 | 32.462 | 49.776 | 1.00 24.18 | AAAA |
| ATOM | 412 | | | O A | | 47.012 47.766 | 32.512 33.862 | 48.390 48.405 | 1.00 24.24 | AAAA |
| ATOM | 413 | | | O A | | 46.473 | 31.070 | 50.393 | 1.00 24.11 1.00 23.69 | AAAA |
| ATOM | 414 | | |) A | | 47.545 | 30.680 | 50.839 | 1.00 24.13 | AAAA |
| ATOM | 415 | | | A A | | 45.381 | 30.325 | 50.422 | 1.00 23.36 | AAAA |
| ATOM | 416 | | | A A | 52 | 45.419 | 28.972 | 50.952 | 1.00 23.64 | AAAA AAAA |
| ATOM | 417 | CB | | AA | 52 | 44.012 | 28.405 | | 1.00 23.86 | AAAA |
| ATOM | 418 | C · | | AA | 52 | 46.260 | 28.145 | 49.994 | 1.00 23.58 | AAAA |
| MOTA | 419 | 0 | AL | A A | 52 | 46.240 | 28.383 | 48.806 | 1.00 24.52 | AAAA |
| MOTA | 420 | N | THE | R A | 53 | 47.009 | 27.185 | 50.501 | 1.00 24.41 | AAAA |
| ATOM | 421 | CA | THE | 8 A | 53 | 47.815 | 26.352 | 49.628 | 1.00 26.26 | AAAA |
| ATOM | 422 | CB | THE | | 53 | 48.933 | 25.642 | 50.405 | 1.00 26.37 | AAAA |
| MOTA | 423 | | 1 THE | | 53 | 48.355 | 24.763 | 51.375 | 1.00 26.51 | AAAA |
| ATOM | 424 | CG: | | | 53 | 49.810 | 26.648 | 51.106 | 1.00 24.48 | AAAA |
| MOTA | 425 | C | THE | | 53 | 46.889 | 25.299 | 49.034 | 1.00 27.63 | AAAA |
| ATOM | 426 | 0 | THE | | 53 | 45.870 | 24.982 | 49.620 | 1.00 29.22 | AAAA |
| MOTA | 427 428 | N CA | LYS | | 54 | 47.240 | 24.776 | | 1.00 29.31 | AAAA |
| ATOM ATOM | 429 | CB | LYS | | 54 54 | 46.450 47.249 | 23.752 23.182 | 47.189 | 1.00 30.61 | AAAA |
| ATOM | 430 | CG | LYS | | 54. | | 22:020 | 46.015 45.304 | 1.00 31.68 | AAAA |
| ATOM | 431 | CD | LYS | | 54 | 45.449 | 22.464 | 44.417 | 1.00 34.38 1.00 36.00 | AAAA |
| ATOM | 432 | CE | LYS | | 54 | 45.943 | 22.850 | 43.025 | 1.00 37.55 | AAAA AAAA |
| ATOM | 433 | NZ | LYS | | 54 | 46.425 | 21.664 | 42.236 | 1.00 37.57 | AAAA |
| MOTA | 434 | C | LYS | A | 54 | 46.127 | 22.640 | 48.170 | 1.00 31.26 | AAAA |
| MOTA | 435 | 0 | LYS | Α | 54 | 45.025 | 22.097 | 48.176 | 1.00 31.72 | AAAA |
| MOTA | 436 | N | GLU | | 55 | 47.102 | 22.312 | 49.006 | 1.00 31.88 | AAAA |
| MOTA | 437 | CA | GLU | | 55 | 46.961 | 21.260 | 50.011 | 1.00 32.29 | AAAA |
| MOTA | 438 | CB | GLU | | 55 | 48.266 | 21.089 | 50.778 | 1.00 34.43 | AAAA |
| MOTA | 439 | CG | GLU | | 55 | 48.265 | 19.901 | 51.706 | 1.00 38.39 | AAAA |
| MOTA | 440 | CD | GLU | | 55 | 49.513 | 19.839 | 52.584 | 1.00 41.46 | AAAA |
| MOTA | 441 442 | OE1 OE2 | | | 55 55 | 49.745 | 18.770 | 53.200 | 1.00 43.30 | - AAAA |
| ATOM ATOM | 443 | C | GLU | | 55 | 50.245 45.851 | 20.859 21.555 | 52.672 51.013 | 1.00 42.45 | AAAA |
| ATOM | 444 | Ö | GLU | | 55 | 45.048 | 20.681 | 51.332 | 1.00 30.43 1.00 30.59 | AAAA AAAA |
| ATOM | 445 | N | GLU | | 56 | 45.822 | 22.782 | 51.532 | 1.00 28.23 | AAAA |
| ATOM | 446 | CA | GLU | | 56 | 44.812 | 23.164 | 52.488 | 1.00 27.69 | AAAA |
| ATOM | 447 | CB | GLU | A | 56 | 45.078 | 24.588 | 52.989 | 1.00 27.90 | AAAA |
| MOTA | 448 | CG | GLU | A | 56 | 46.434 | 24.721 | 53.670 | 1.00 26.64 | AAAA |
| MOTA | 449 | CD | GLU | Α | 56 | 46.769 | 26.135 | 54.098 | 1.00 26.35 | AAAA |
| ATOM | 450 | OE1 | GLU | A | 56 | 46.615 | 27.057 | 53.265 | 1.00 25.12 | AAAA |
| MOTA | 451 | OE2 | GLU | | 56 | 47.213 | 26.315 | 55.255 | 1.00 25.70 | AAAA |
| ATOM | 452 | C | GLU | | 56 | 43.408 | 23.043 | 51.914 | 1.00 26.99 [.] | AAAA |
| ATOM | 453 | 0 | GLU | | 56 | 42.495 | 22.574 | 52.588 | 1.00 26.25 | AAAA |
| ATOM | 454 | N | LEU | | 57 | 43.252 | 23.447 | 50.659 | 1.00 27.26 | AAAA |
| ATOM | 455 | CA | LEU | | 57 | 41.965 | 23.389 | 49.967 | 1.00 27.17 | AAAA |
| ATOM | 456 | CB | LEU | | 57· | 42.077 | 24.063 | 48.596 | 1.00 26.62 | AAAA |
| ATOM | 457 450 | CG | LEU | | 57 57 | 42.491 | 25.545 | 48.656 | 1.00 27.64 | AAAA |
| ATOM | 458 150 | | | | 57 57 | 42.770 | 26.108 | 47.269 | 1.00 26.66 | AAAA |
| ATOM | 459 460 | CDZ | LEU | | 57 | 41.389 41.552 | 26.341 | 49.349 49.796 | 1.00 26.92 1.00 27.26 | AAAA |
| ATOM ATOM | 460 461 | ō | LEU | | 57 | 40.363 | 21.946 21.612 | 49.736 | 1.00 27.26 | AAAA AAAA |
| ATOM | 462 | N | LEU | | 58 | 42.547 | 21.012 | 49.641 | 1.00 27.33 | AAAA |
| | 04 | | | •• | | 34.531 | ~4.000 | - | 2732 | WWW |



Figure 19-8

| ATOM | 463 | CA | LEU A | 58 | 42.293 | 19.675 | 49.457 | 1.00 26.10 | AAAA |
|-------------------|------|-----|---------|------------|--------|--------|--------|--------------|-------|
| ATOM | 464 | | LEU A | 58 | 43.486 | | 48.794 | 1.00 25.43 | AAAA |
| | | | | | | | | | |
| ATOM | 465 | CG | LEU A | 58 | 43.623 | 19.577 | 47.385 | 1.00 26.66 | AAAA |
| MOTA | 466 | CD: | L LEU A | 58 | 44.760 | 18.884 | 46.705 | 1.00 27.12 | AAAA |
| | 467 | | LEU A | 58 | 42.334 | 19.355 | 46.600 | 1.00 26.43 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 468 | С | LEU A | 58 | 41.938 | 18.956 | 50.731 | 1.00 25.79 | AAAA |
| ATOM | 469 | 0 | LEU A | 58 | 41.648 | 17.763 | 50.692 | 1.00 26.50 | AAAA |
| | | | | | | | | 1.00 24.91 | |
| ATOM | 470 | N | LEU A | 59 | 41.977 | 19.666 | 51.858 | | AAAA |
| ATOM | 471 | CA | LEU A | 59 | 41.595 | 19.070 | 53.136 | 1.00 25.15 | AAAA |
| ATOM | 472 | CB | LEU A | 59 | 41.958 | 19.991 | 54.322 | 1.00 25.44 | AAAA |
| | | | | | | | | | |
| ATOM | 473 | CG | LEU A | 59 | 43.423 | 20.280 | 54.710 | 1.00 24.67 | AAAA |
| ATOM | 474 | CD1 | LEU A | 59 | 43.502 | 21.461 | 55.652 | 1.00 23.70 | AAAA |
| ATOM | 475 | | LEU A | 59 | 44.044 | 19.044 | 55.357 | 1.00 24.08 | AAAA |
| | | | | | | | | | |
| ATOM | 476 | Ç | LEU A | 59 | 40.074 | 18.870 | 53.090 | 1.00 25.41 | AAAA |
| ATOM | 477 | 0 | LEU A | 59 | 39.503 | 18.266 | 53.993 | 1.00 25.88 | AAAA |
| | 478 | N | PHE A | 60 | 39.436 | 19.392 | 52.031 | 1.00 25.05 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 479 | CA | PHE A | 60 | 37.983 | 19.276 | 51.823 | 1.00 24.11 | AAAA |
| ATOM | 480 | CB | PHE A | 60 | 37.250 | 20.476 | 52.440 | 1.00 21.80 . | AAAA |
| | 481 | CG | PHE A | 60 | 35.778 | 20.534 | 52.098 | 1.00 20.07 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 482 | CD1 | PHE A | 6 0 | 34.917 | 19.501 | 52.462 | 1.00 19.27 | AAAA |
| MOTA | 483 | CD2 | PHE A | 60 | 35.249 | 21.628 | 51.399 | 1.00 19.82 | AAAA |
| | 484 | | PHE A | 60 | 33.550 | 19.557 | 52.136 | 1.00 19.26 | AAAA |
| atom | | | | | | | | | |
| ATOM | 485 | CE2 | PHE A | 60 | 33.890 | 21.688 | 51.071 | 1.00 17.45 | AAAA |
| MOTA | 486 | CZ | PHE A | 60 | 33.042 | 20.652 | 51.440 | 1.00 17.92 | AAAA |
| | 487 | C | PHE A | 60 | 37.557 | 19.139 | 50.345 | 1.00 24.02 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 488 | 0 | PHE A | 60 | 36.846 | 18.201 | 49.974 | 1.00 23.27 | AAAA |
| MOTA | 489 | N | HIS A | 61 | 37.982 | 20.079 | 49.511 | 1.00 24.40 | AAAA |
| | 490 | CA | HIS A | 61 | 37.626 | 20.053 | 48.099 | 1.00 25.04 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 491 | CB | HIS A | 61 | 37.768 | 21.449 | 47.494 | 1.00 24.19 | AAAA |
| ATOM | 492 | CG | HIS A | 61 | 36.744 | 22.429 | 47.979 | 1.00 24.44 | AAAA |
| ATOM | 493 | | HIS A | 61 | 35.429 | 22.559 | 47.683 | 1.00 24.12 | AAAA |
| | | | | | | | | | |
| MOTA | 494 | NDT | HIS A | 61 | 37.038 | 23.444 | 48.864 | 1.00 24.36 | AAAA |
| ATOM | 495 | CE1 | HIS A | 61 | 35.952 | 24.159 | 49.089 | 1.00 23.18 | AAAA |
| ATOM | 496 | | HIS A | 61 | 34.962 | 23.643 | 48.385 | 1.00 23.91 | AAAA |
| | | | | | | | 47.253 | | AAAA |
| ATOM | 497 | С | HIS A | 61 | 38.416 | 19.054 | | 1.00 25.60 | |
| ATOM | 498 | 0 | HIS A | 61 | 39.596 | 18.805 | 47.498 | 1.00 26.94 | AAAA |
| ATOM | 499 | N | THR A | 62 | 37.754 | 18.496 | 46.244 | 1.00 26.68 | AAAA |
| | | | | | 38.369 | 17.522 | 45.333 | 1.00 28.17 | AAAA |
| ATOM | 500 | CA | THR A | 62 | | | | | |
| ATOM | 501 | CB | THR A | 62 | 37.290 | 16.695 | 44.614 | 1.00 28.15 | AAAA |
| ATOM | 502 | OG1 | THR A | 62 | 36.544 | 17.541 | 43.731 | 1.00 28.10 | AAAA |
| | 503 | | THR A | 62 | 36.334 | 16.094 | 45.629 | 1.00 28.24 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 504 | С | THR A | 62 | 39.226 | 18.217 | 44.278 | 1.00 29.28 | AAAA |
| MOTA | 505 | 0 | THR A | 62 | 38.876 | 19.286 | 43.792 | 1.00 29.52 | AAAA |
| ATOM | 506 | N | GLU A | 63 | 40.344 | 17.606 | 43.912 | 1.00 31.33 | AAAA |
| | | | | | | | | | AAAA |
| ATOM | 507 | CA | GLU A | 63 | 41.249 | 18.202 | 42.928 | 1.00 32.42 | |
| ATOM | 508 | CB | GLU A | - 63 | 42.333 | 17.219 | 42.536 | 1 00 34.37 | AAAA |
| ATOM | 509 | CG | GLU A | 63 | 43.304 | 16.869 | 43.609 | 1 00 37.20 | AAAA |
| | | | | | | 16.022 | 43.052 | 1 00 38.79 | AAAA |
| MOTA | 510 | CD | GLU A | 63 | 44.427 | | | | |
| ATOM | 511 | OE1 | GLU A | 63 | 45.100 | 16.499 | 42.097 | 1.00 37.96 | AAAA |
| MOTA | 512 | OE2 | GLU A | 63 | 44.619 | 14.892 | 43.564 | 1.00 39.68 | AAAA |
| | | | | | | | 41.639 | 1.00 31.96 | AAAA |
| ATOM | 513 | С | GLU A | 63 | 40.607 | | | | |
| ATOM | 514 | 0 | GLU A | 63 | 40.824 | 19.816 | | 1.00 32.10 | AAAA |
| MOTA | 515 | N | ASP A | 64 | 39.845 | 17.814 | 40.998 | 1.00 31.52 | AAAA |
| | | | | | 39:204 | 18.165 | 39.753 | 1.00 31.36 | AAAA |
| ATOM | 516 | CA | ASP A | 64 | | | | | |
| MOTA | 517 | CB | ASP A | 64 | 38.301 | 17.018 | 39.295 | 1.00 33.99 | AAAA |
| ATOM | 518 | CG | ASP A | 64 | 37.213 | 16.694 | 40.302 | 1.00 37.38 | AAAA |
| | | | | | 36.375 | 15.801 | 40.027 | 1.00 39.80 | AAAA |
| MOTA | 519 | | ASP A | 64 | | | | | |
| MOTA | 520 | OD2 | ASP A | 64 | 37.188 | 17.332 | 41.374 | 1.00 38.67 | AAAA |
| ATOM | 521 | С | ASP A | 64 | 38.412 | 19.465 | 39.902 | 1.00 30.02 | AAAA |
| | | | | 64 | 38.462 | 20.331 | 39.026 | 1.00 30.47 | AAAA |
| Mota | 522 | 0 | ASP A | | | | | | |
| ATOM | 523 | N | TYR A | 65 | 37.695 | 19.608 | 41.012 | 1.00 27.51 | AAAA |
| ATCM | 524 | CA | TYR A | 65 | 36.918 | 20.814 | 41.248 | 1.00 26.03 | AAAA |
| | | | | 65 | 36.010 | 20.654 | 42.467 | 1,00 25.42 | AAAA |
| ATOM | 525 | CB | TYR A | | | | | | |
| MOTA | 526. | CG | TYR A | 65 | 35.339 | 21.946 | 42.866 | 1.00 24.90 | AAAA |
| ATOM | 527 | CD1 | TYR A | 65 | 34.525 | 22.636 | 41.964 | 1.00 25.04 | AAAA |
| • | | | TYR A | 65 | 33.914 | 23.823 | 42.308 | 1.00 25.01 | AAAA. |
| atom _. | 528 | CT | TIN | 0.5 | 23.314 | 22.022 | | | |
| | | | | | • | | | | • |

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Figure 19-9

| ATOM | 529 | CD | 2 TYF | R A | 65 | | 35.525 | 22.486 | 44.136 | 1.00 | 24.65 | AAAA |
|--------------|-------------|----------|------------|-------|------------|---|------------------|------------------|------------------|------|----------------|--------------|
| ATOM · | 530 | CE. | 2 TYF | 8 · A | 55 | | 34.920 | 23.677 | 44.497 | | 25.86 | AAAA |
| MOTA | 531 | CZ | TYF | A S | 65 | | 34.110 | 24.349 | | | 26.69 | AAAA |
| ATOM | 532 | OH | TYR | A 5 | 65 | | 33.499 | | | | 27.20 | AAAA |
| MOTA | 533 | С | TYR | l A | 65 | | 37.814 | | 41.464 | 1.00 | 24.91 | AAAA |
| MOTA | 534 | 0 | TYR | A S | 65 | • | 37.460 | | 41.096 | | 25.62 | AAAA |
| ATOM | 535 | N | _ ILE | · A | 66 | | 38.965 | | | 1.00 | 23.20 | AAAA |
| MOTA | 536 | CA | ILE | · A | 66 | | 39.877 | 22.902 | 42.328 | 1.00 | 22.33 | AAAA |
| MOTA | 537 | CB | ILE | · A | 66 | | 40.924 | 22.520 | 43.402 | 1.00 | 21.45 | AAAA |
| MOTA | 538 | CG | 2 ILE | A | 66 | | 41.927 | 23.652 | 43.617 | 1.00 | 20.00 | AAAA |
| MOTA | 539 | | LILE | | 66 | - | 40.220 | 22.289 | 44.729 | 1.00 | 20.16 | AAAA |
| MOTA | 540 | | LILE | | 66 | | 39.528 | 23.523 | 45.228 | 1.00 | 19.68 | AAAA |
| MOTA | 541 | С | ILE | | 66 | | 40.558 | 23.261 | 41.023 | 1.00 | 22.68 | AAAA |
| MOTA | 542 | 0 | ILE | | 66 | | 40.636 | | | 1.00 | 23.19 | AAAA |
| MOTA | 543 | N | ASN | | 67 | | 41.036 | | | | 22.96 | AAAA |
| MOTA | 544 | CA | ASN | | 67 | | 41.698 | | | | 23.92 | AAAA |
| ATOM | 545 | СВ | ASN | | 67 | - | 42.292 | | 38.395 | | 24.24 | AAAA |
| MOTA | 546 | CG | ASN | | 67 | • | 43.344 | | 39.289 | | 23.38 | AAAA |
| MOTA | 547 | | ASN | | 67 | | 44.196 | | 39.859 | | 23.47 | AAAA |
| MOTA | 548 | | ASN | | 67. | | 43.290 | | 39.392 | | 23.20 | AAAA |
| MOTA | 549 | C | ASN | | 67 | | 40.717 | | 38.063 | | 23.82 | AAAA |
| MOTA | 550 551 | O N | ASN THR | | · 67 68 | | 41.123 | | 37.204 | | 24.63 | AAAA |
| MOTA MOTA | 552 | CA | THR | | 68 | | 39.427 38.428 | | 38.213 37.343 | | 24.08 | AAAA |
| ATOM | 553 | CB | THR | | 68 | | 37.030 | | 37.525 | | 25.28 24.55 | AAAA |
| ATOM | 554 | | THR | | 68 | | 37.090 | | 37.258 | | 24.55 | AAAA |
| ATOM | 555 | CG2 | | | 68 | | 36.049 | | 36.564 | | 23.58 | AAAA AAAA |
| ATOM | 556 | c | THR | | 68 | | 38.322 | 25.023 | 37.664 | | 26.31 | AAAA |
| ATOM | 557 | ō | THR | | 68 | | 38.114 | 25.854 | 36.771 | | 26.69 | AAAA |
| ATOM | 558 | N | LEU | Α | 69 | | 38.462 | 25.351 | 38.945 | | 26.59 | AAAA |
| MOTA | 559 | CA | LEU | A | 69 | | 38.381 | 26.729 | 39.378 | | 27.05 | AAAA |
| ATOM | 560 | CB | LEU | A | 69 | | 38.321 | 26.807 | 40.904 | 1.00 | 27.15 | AAAA |
| MOTA | 561 | CG | LEU | | 69 | | 37.003 | 26.397 | 41.551 | 1.00 | 25.68 | AAAA |
| MOTA | 562 | | LEU | | 69 | | 37.088 | 26.491 | 43.062 | | 26.30 | AAAA |
| ATOM | 563 | | LEU | | 69 | | 35.933 | 27.316 | 41.044 | | 26.14 | AAAA |
| ATOM | 564 | C | LEU | | 69 | | 39.570 | 27.508 | 38.867 | | 28.44 | AAAA |
| MOTA | 565 566 | O | LEU | | 69 70 | | 39.425 | 28.619 | 38.356 | | 28.59 | AAAA |
| MOTA | 566 567 | N CA | MET MET | | 70 70 | | 40.748 | 26.914 | 39.009 | | 29.31 | AAAA |
| ATOM ATOM | 568 | CB | MET | | 70 | | 41.981 43.160 | 27.536 26.692 | 38.571 39.044 | | 29.89 31.04 | AAAA |
| MOTA | 569 | CG | MET | | 70 | | 43.164 | 26.528 | 40.562 | | 31.79 | AAAA AAAA |
| ATOM | 570 | SD | | A | 70 | | 44.608 | 25.684 | 41.183 | | 32.58 | AAAA |
| ATOM | 571 | CE | MET | | 70 | | 45.859 | 26.820 | 40.670 | | 30.82 | AAAA |
| MOTA | 572 | С | MET | | 70 | | 42.017 | 27.723 | 37.057 | | 30.36 | AAAA |
| ATOM | 573 | 0 | MET | A | 70 | | 42.462 | 28.769 | 36.559 | | 30.18 | AAAA |
| MOTA | . 574 . | - N | GLU | A | 71 | | 41.538 | 26.719 | 36.328 | 1.00 | 30.34 | AAAA |
| MOTA | 575 | CA | GLU | А | 71 | | 41.519 | 26.795 | 34.874 | 1.00 | 30.73 | AAAA |
| ATOM | 576 | CB | GLU | | 71 | | 41.140 | 25.442 | 34.266 | 1.00 | 33.47 | AAAA |
| MOTA | 57 7 | CG | GLU | | 71 | | 41.122 | 25.430 | 32.731 | | 37.11 | AAAA |
| ATOM | 578 | CD | GLU | | 71 | | 42.513 | 25.676 | 32.093 | | 40.49 | AAAA |
| ATOM | 579 | | GLU | | 71 | | 42.570 | 25.798 | 30.844 | | 41.95 | AAAA |
| ATOM | 580 | | GLU | | 71 | | 43.541 | 25.738 | 32.825 | | 40.74 | AAAA |
| ATOM | 581 | C | GLU . | | 71 | | 40.537 | 27.851 | 34.392 | | 29.78 | AAAA |
| MOTA | 582 | 0 | GLU . | | 71 | | 40.852 | 28.642 | 33.508 | | 27.82 | AAAA |
| MOTA | 583 | N | ALA . | | 72 | | 39.352 | 27.855 | 34.992 | | 29.85 | AAAA |
| ATOM | 584 585 | CA CB | ALA . | | 72 72 | | 38.296 | 28.790 | 34.635 | | 29.88 | AAAA |
| ATOM | 58 6 | | ALA . | | 72 | | 37.022 38.667 | 28.432 30.238 | 35.374 34.907 | | 29.07 30.78 | AAAA |
| ATOM ATOM | 587 | | ALA I | | 72 | | 38.359 | 31.122 | 34.108 | | 31.27 | AAAA AAAA |
| ATOM | 588 | | GLU . | | 73 | | 39.336 | 30.491 | 36.023 | | 31.27 | AAAA AAAA |
| ATOM | 589 | | GLU : | | 73 | | 39.710 | 31.856 | 36.346 | | 31.65 | AAAA |
| ATOM | 590 | | GLU 2 | | 73 | | 40.243 | 31.954 | 37.785 | | 30.52 | AAAA |
| ATOM | 591 | | GLU Z | | 73 | | 40.643 | 33.370 | 38.198 | 1.00 | | AAAA |
| MOTA | 592 | | GLU A | | 73 | | 41.076 | 33.484 | 39.651 | 1.00 | | AAAA |
| ATOM | 593 | | GLU A | | 73 | | 40.239 | 33.260 | 40.546 | 1.00 | | AAAA |
| ATOM | 594 | OE2 | GLU A | A. | 73 | | 42.258 | 33.795 | 39.906 | 1.00 | | AAAA |
| • | | | | | | | | | - | | | |

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| > mow | 595 | С | GLU A | 73 | 40.726 | 32.461 | 35.378 | 1.00 33.54 | 2222 |
|-------|------|-----|---------------|------------|--------|--------|--------|------------|--------|
| ATOM | 596 | | | | | | | | AAAA |
| ATOM | | 0 | GLU A | 73 | 40.456 | 33.499 | 34.767 | 1.00 34.93 | AAAA |
| ATOM | 597 | N | ARG A | 74 | 41.885 | 31.832 | 35.214 | 1.00 34.35 | AAAA |
| MOTA | 598 | CA | ARG A | 74 | 42.890 | 32.428 | 34.334 | 1.00 36.04 | AAAA |
| ATOM | 599 | CB | ARG A | 74 | 44.238 | 31.710 | 34.482 | 1.00 36.92 | AAAA |
| -MOTA | 600 | CG | ARG A | 74 | 44.327 | 30.313 | 33.923 | 1.00 38.14 | AAAA |
| ATOM | 601 | CD | ARG A | 74 | 45.508 | 29.589 | 34.543 | 1.00 39.55 | AAAA |
| ATOM | 602 | NE | ARG A | 74 | 45.893 | 28.404 | 33.785 | 1.00 42.02 | AAAA |
| ATOM | 603 | CZ | ARG A | 74 | 46.632 | 28.436 | 32.675 | 1.00 42.69 | AAAA |
| | 604 | | ARG A | 74 | 47.071 | 29.593 | 32.191 | 1.00 42.76 | AAAA |
| ATOM | | | | | | 27.309 | 32.046 | | |
| ATOM | 605 | | ARG A | 74 | 46.933 | | | 1.00 42.92 | AAAA |
| ATOM | 606 | C | ARG A | 74 | 42.476 | 32.532 | 32.864 | 1.00 36.56 | AAAA |
| ATOM | 607 | 0 | ARG A | 74 | 42.842 | 33.493 | 32.187 | 1.00 37.73 | AAAA |
| ATOM | 608 | N | SER A | 75 | 41.711 | 31.567 | 32.367 | 1.00 36.60 | AAAA |
| ATOM | 609 | CA | SER A | 75 | 41.248 | 31.622 | 30.987 | 1.00 36.82 | AAAA |
| MOTA | 610 | CB | SER A | 75 | 40.916 | 30.218 | 30.478 | 1.00 36.10 | - AAAA |
| ATOM | 611 | OG | SER A | 75 | 39.736 | 29.723 | 31.083 | 1.00 36.39 | AAAA |
| MOTA | 612 | С | SER A | 75 | 39.980 | 32.476 | 31.001 | 1.00 36.90 | AAAA |
| ATOM | 613 | 0 | SER A | 75 | 39.401 | 32.791 | 29.963 | 1.00 36.25 | AAAA |
| ATOM | 614 | N | GLN A | 76 | 39.568 | 32.845 | 32.208 | 1.00 37.62 | AAAA |
| ATOM | 615 | CA | GLN A | 76 | 38.368 | 33.639 | 32.427 | 1.00 37.92 | AAAA |
| MOTA | 616 | CB | GLN A | 76 | 38.613 | 35.100 | 32.049 | 1.00 38.23 | AAAA |
| ATOM | 617 | CG | GLN A | 76 | 37.630 | 36.048 | 32.717 | 1.00 40.67 | AAAA |
| ATOM | 618 | CD | GLN A | 76 | 37.929 | 36.298 | 34.199 | 1.00 41.40 | AAAA |
| ATOM | 619 | | GLN A | 76 | 38.226 | 35.379 | 34.973 | 1.00 40.79 | AAAA |
| | 620 | | GLN A | 76 | 37.833 | 37.556 | 34.597 | 1.00 42.32 | AAAA |
| ATOM | 621 | C | GLN A | 76 | 37.223 | 33.064 | 31.600 | 1.00 37.75 | AAAA |
| ATOM | | | | | 36.521 | 33.789 | 30.901 | 1.00 37.73 | |
| ATOM | 622 | 0 | GLN A | 76 | | | | | AAAA |
| ATOM | 623 | N | SER A | 77 | 37.045 | 31.749 | 31.685 | 1.00 37.52 | AAAA |
| ATOM | 624 | CA | SER A | 77 | 35.990 | 31.061 | 30.950 | 1.00 37.75 | AAAA |
| ATOM | 625 | CB | SER A | 77 | 36.537 | 30.440 | 29.664 | 1.00 37.90 | AAAA |
| MOTA | 626 | OG | SER A | 77 | 36.851 | 31.441 | 28.724 | 1.00 40.32 | AAAA |
| MOTA | 627 | С | SER A | 77 | 35.338 | 29.960 | 31.757 | 1.00 37.55 | AAAA |
| ATOM | 628 | 0 | SER A | 7 7 | 35.790 | 29.620 | 32.846 | 1.00 36.81 | AAAA |
| ATOM | 629 | N | VAL A | 78 | 34.264 | 29.412 | 31.198 | 1.00 37.82 | AAAA |
| MOTA | 630 | CA | VAL A | 78 | 33.538 | 28.309 | 31.812 | 1.00 37.99 | AAAA |
| ATOM | 631 | CB | VAL A | 78 | 32.027 | 28.514 | 31.715 | 1.00 37.19 | AAAA |
| ATOM | 632 | CG1 | VAL A | 78 | 31.310 | 27.439 | 32.497 | 1.00 36.84 | AAAA |
| ATOM | 633 | CG2 | VAL A | 78 | 31.662 | 29.906 | 32.201 | 1.00 37.60 | AAAA |
| ATOM | 634 | С | VAL A | 78 | 33.918 | 27.089 | 30.976 | 1.00 38.28 | AAAA |
| ATOM | 635 | 0 | VAL A | 78 | 33.497 | 26.959 | 29.819 | 1.00 39.18 | AAAA |
| ATOM | 636 | N | PRO A | 79 | 34.734 | 26.187 | 31.537 | 1.00 37.69 | AAAA |
| ATOM | 637 | CD | PRO A | 79 | 35.347 | 26.167 | 32.869 | 1.00 37.65 | AAAA |
| ATOM | 638 | CA | PRO A | 79 | 35.146 | 24.998 | 30.797 | 1.00 37.54 | AAAA |
| ATOM | 639 | CB | PRO A | 79 | 36.127 | 24.325 | 31.759 | 1.00 37.45 | AAAA |
| ATOM | 640 | CG | PRO A | 79 | 36.655 | 25.489 | 32.557 | 1.00 37.65 | AAAA |
| ATOM | 641 | c | PRO A | 79 | 33.980 | 24.089 | 30.434 | 1.00 37.20 | AAAA |
| | 642 | ō | PRO A | 79 | 32.958 | 24.050 | 31.120 | 1.00 36.43 | AAAA |
| ATOM | 643 | N | LYS A | 80 | 34.154 | 23.363 | 29.338 | 1.00 37.42 | AAAA |
| ATOM | 644 | CA | | | | 22.423 | 28.855 | 1.00 37.35 | |
| ATOM | | | LYS A | 80 | 33.160 | 21.586 | 27.725 | 1.00 37.33 | |
| ATOM | 645 | CB | LYS A | 80 | 33.757 | | 27.723 | 1.00 37.99 | AAAA |
| ATOM | 646 | CG | LYS A | 80 | 32.928 | 20.379 | | | AAAA |
| atom | 647 | CD | LYS A | 80 | 31.835 | 20.710 | 26.286 | 1.00 39.07 | AAAA |
| atom | .648 | CE | LYS A | 80 | 31.320 | 19.402 | 25.688 | 1.00 40.43 | AAAA |
| MOTA | 649 | NZ | LYS A | 80 | 30.498 | 19.543 | 24.450 | 1.00 40.48 | AAAA |
| ATOM | 650 | С | LYS A | 80 | 32.752 | 21.515 | 30.003 | 1.00 36.85 | AAAA |
| ATOM | 65,1 | 0 | LYS A | 80 | 33.610 | 20.942 | 30.676 | 1.00 36.56 | AAAA |
| MOTA | 652 | N | GLY A | 81 | 31.443 | 21.408 | 30.217 | 1.00 35.94 | AAAA |
| ATOM | 653 | CA | GLY A | 81 | 30.903 | 20,570 | 31.268 | 1.00 35.48 | AAAA |
| ATOM | 654 | С | GLY A | 81 | 31.110 | 21.054 | 32.695 | 1.00 35.23 | AAAA |
| TOM | 655 | 0 | GLY A | 81 | 30.749 | 20.355 | 33.644 | 1.00 35.46 | AAAA |
| TOM | 656 | N | ALA A | 82 | 31.677 | 22.241 | 32.867 | 1.00 35.17 | AAAA |
| TOM | 657 | CA | ALA A | 82 | 31.919 | 22.743 | 34.213 | 1.00 35.02 | AAAA |
| ATOM | 658 | CB | ALA A | 82 | 33.076 | 23.743 | 34.208 | 1.00 35.13 | AAAA |
| ATOM | 659 | c | ALA A | 82 | 30.674 | 23.378 | 34.797 | 1.00 34.39 | AAAA |
| | 660 | 0 | ALA A | 82 | 30.451 | 23.332 | 36.001 | 1.00 33.82 | AAAA |
| MOTA | 000 | • | | ~ ** | 30.931 | 27.322 | | | |
| | | | 6 From | _ | | | | | |

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Figure 19-11

| MOTA | 661 | . N | ARC | a A | . 83 | 2 | 9.858 | 23,960 | 33.932 | 1.00 | 34.77 | AAAA |
|--------------|------------|----------|----------------|-----|-----------|-----|----------------|------------------|------------------|------|----------------|----------------|
| ATOM | 662 | CA | ARG | S A | . 83 | . 2 | 8.637 | | | | 35.34 | |
| ATOM | 663 | СВ | ARG | A | . 83 | 2 | 7.899 | 25.180 | | | 36.26 | |
| ATOM | 664 | CG | ARG | A | . 83 | 2 | 7.045 | 26.395 | | | 37.09 | |
| ATOM | 665 | CD | ARG | A | . 83 | 2 | 6.209 | 26.141 | 34.686 | | 37.48 | |
| ATOM | 666 | NE | ARG | A | 83 | 2 | 5.475 | 27.310 | | | 37.35 | AAAA |
| MOTA | 667 | CZ | ARG | A | 83 | 2 | 4.711 | 27.311 | 36.218 | 1.00 | 37.77 | AAAA |
| MOTA | 668 | NH: | 1 ARG | | | 2 | 4.606 | | | 1.00 | 37.29 | |
| ATOM | 669 | NH. | 2 ARG | A | . 83 | 2 | 4.040 | 28.401 | 36.568 | | 38.34 | |
| ATOM | 670 | | ARG | | | 2 | 7.739 | 23.603 | 35.065 | 1.00 | 36.30 | AAAA |
| MOTA | 671 | | ARG | | 83 | 2 | 7.232 | 23.854 | 36.154 | | 36.17 | AAAA |
| MOTA | 672 | | GLU | | 84 | | 7.565 | | | 1.00 | 37.19 | AAAA |
| MOTA | 673 | CA | GLU | | 84 | | 6.721 | | | | 37.80 | AAAA . |
| ATOM | 674 | CB | GLU | | 84 | | 6.466 | | | | 40.55 | AAAA |
| ATOM | 675 | CG | GLU | | 84 | | 5.643 | 19.171 | | | 43.12 | AAAA |
| MOTA | 676 | CD | GLU | | 84 | | 5.362 | 18.268 | | | 44.98 | AAAA |
| ATOM | 677 | | GLU | | 84 | | 4.573 | 17.301 | | | 46.36 | AAAA |
| ATOM | 678 | OE2 | | | 84 | | 5.937 | 18.532 | | | 44.94 | AAAA |
| ATOM | 679 | C | GLU | | 84 | | 7.290 | 20.657 | | | 37.07 | AAAA |
| ATOM | 680 | O N | GLU | | 84 | | 6.642 | 20.555 | | | 36.17 | AAAA |
| MOTA | 681 682 | N CA | LYS | | 85 | | 8.506 | 20.152 | | | 36.23 | AAAA |
| MOTA MOTA | 683 | CB | LYS LYS | | 85 85 | | 9.202 | 19.412 | | | 35.36 | AAAA |
| MOTA | 684 | CG | LYS | | 85 | | 0.449 1.394 | 18.761 | | | 36.96 | AAAA |
| ATOM | 685 | CD | LYS | | 85 | | 0.995 | 18.158 16.766 | | | 39.04 | AAAA |
| ATOM | 686 | CE | LYS | | 85 | | 1.508 | 15.719 | | | 40.59 41.88 | AAAA |
| ATOM | 687 | NZ | LYS | | 85 | | 2.998 | 15.817 | | | 42.00 | AAAA |
| MOTA | 688 | C | LYS | | 85 | | 9.620 | 20.202 | 38.289 | | 33.86 | AAAA AAAA |
| ATOM | 689 | 0 | LYS | | 85 | | 5.576 | 19.679 | 39.404 | | 33.82 | AAAA |
| ATOM | 690 | N | TYR | Α | 86 | | 0.014 | 21.458 | 38.097 | | 32.06 | AAAA |
| MOTA | 691 | CA | TYR | Α | 86 | 30 | 0.514 | 22.279 | 39.194 | | 29.44 | AAAA |
| ATOM | 692 | CB | TYR | A | 86 | 31 | 1.956 | 22.683 | 38.875 | | 29.97 | AAAA |
| MOTA | 693 | CG | TYR | | 86 | 32 | 2.872 | 21.496 | 38.621 | 1.00 | 29.99 | AAAA |
| MOTA | 694 | | TYR | | 86 | | .281 | 20:666 | 39.666 | | 29.24 | AAAA |
| ATOM . | 695 | | TYR | | 86 | | .126 | 19.582 | 39.437 | 1.00 | 29.85 | AAAA |
| MOTA | 696 | CD2 | | | 86 | | .329 | 21.204 | 37.329 | | 30.16 | AAAA |
| MOTA | 697 | CE2 | TYR | | 86 | | .173 | 20.118 | 37.087 | | 29.61 | AAAA |
| ATOM ATOM | 698 699 | CZ OH | TYR TYR | | 86 | | .570 | 19.313 | 38.148 | | 29.79 | AAAA |
| ATOM | 700 | C | TYR | | 86 86 | | .705 | 18.253 23.509 | 37.923 39.572 | | 29.48 | AAAA |
| ATOM | 701 | o. | TYR | | 86 | | .052 | 24.202 | 40.524 | | 27.81 27.56 | AAAA |
| ATOM | 702 | Ŋ | ASN | | 87 | | .642 | 23.784 | 38.828 | | 26.60 | AAAA AAAA |
| ATOM | 703 | CA | ASN | | 87 | | .777 | 24.924 | 39.111 | | 26.56 | AAAA |
| ATOM | 704 | СВ | ASN | | 87 | | .172 | 24.772 | 40.508 | | 26.39 | AAAA |
| MOTA | 705 | CG | ASN | Α | 87 | | .863 | 25.544 | 40.684 | | 26.64 | AAAA |
| ATOM | 706 | OD1 | ASN | A | 87 | | .335 | 25.632 | 41.790 | | 26.84 | AAAA |
| ATOM | 707 | ND2 | ASN | A | 87 | 25 | .330 | 26.084 | 39.597 | 1.00 | 26.33 | AAAA |
| ATOM | 708 | C | ASN | | 87 | 28 | .587 | 26.217 | 39.024 | 1.00 | 26.40 | AAAA |
| MOTA | 709 | 0 | ASN . | | 87 | 28 | .430 | 27.129 | 39.832 | 1.00 | 24.80 | AAAA |
| ATOM | ?10 | N | ILE . | | 88 | 29 | .448 | . 26.273 | 38.015 | 1.00 | 27.57 | AAAA |
| MOTA | 711 | CA | ILE . | | 88 | | .330 | 27.409 | 37.767 | | 27.88 | AAAA |
| ATOM | 712 | CB | ILE . | | 88 | | . 817 | 26.932 | 37.648 | | 27.38 | AAAA |
| MOTA | 713 | | ILE ! | | 88 | | . 684 | 27.994 | 36.986 | | 26.34 | AAAA |
| MOTA | 714 | | ILE A | | 88 | | . 354 | 26.543 | 39.026 | | 28.35 | AAAA |
| ATOM | 715 | | ILE A | | 88 | | .356 | 27.671 | 40.042 | | 27.78 | AAAA |
| MOTA | 716 | C | ILE A | | 88 | | .946 | 28.110 | 36.472 | | 29.17 | · AAAA |
| ATOM | 717 | | ILE A | | 88 | | . 530 | 27.469 | 35.515 | | 29.75 | AAAA |
| ATOM | 718 719 | | GLY A | | 89 | | . 092 | 29.429 | 36.443 | | 29.96 | AAAA |
| ATOM | 720 | | GLY 2 | | 89 | | .791 | 30.162 | 35.229 | 1.00 | | AAAA |
| MOTA MOTA | 721 | | GLY ? GLY ? | | 89. 89 | | .430 | 30.805 | 35.242 34.514 | 1.00 | | AAAA |
| ATOM | 722 | | GLY ? | | 90 | | . 177 . 542 | 31.769 30.268 | 36.061 | 1.00 | | AAAA |
| ATOM | 723 | | GLY A | | 90 | | . 221 · | 30.268 | 36.129 | 1.00 | | . AAAA AAAA |
| ATOM | 724 | | GLY ? | | 90 | | . 283 | 32.262 | 36.661 | 1.00 | | AAAA AAAA |
| ATOM | 725 | | GLY ? | | 90 | | . 356 | 32.795 | 36.962 | 1.00 | | AAAA AAAA |
| ATOM | 726 | | TYR A | | 91 | | 112 | 32.873 | 36.768 | 1.00 | | AAAA |
| | | - | • | | _ | | | | | | | 14441 |

| ATOM | 727 | CA | TYR A | 91 | 24.977 | 34.213 | 37.290 | 1.00 31.27 | AAAA |
|------|-------|-----|-------|----|----------|--------|----------------|------------|-------|
| ATOM | 728 | CB | TYR A | 91 | 23.515 | 34.634 | 37.195 | 1.00 31.82 | AAAA |
| | | | | | | | | 1.00 31.81 | |
| ATOM | 729 | CG | TYR A | 91 | 23.169 | 35.825 | 38.047 | | AAAA |
| ATOM | 730 | CD1 | TYR A | 91 | 23.536 | 37.108 | 37.670 | 1.00 32.44 | AAAA |
| | 731 | CE1 | TYR A | 91 | 23.250 | 38.203 | 38.475 | 1.00 31.88 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 732 | CD2 | TYR A | 91 | 22.505 | 35.663 | 39.254 | 1.00 32.63 | AAAA |
| MOTA | 733 | CE2 | TYR A | 91 | 22.215 | 36.754 | 40.068 | 1.00 32.60 | AAAA |
| | 734 | CZ | TYR A | 91 | 22.589 | 38.016 | 39.668 | 1.00 31.59 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 735 | OH | TYR A | 91 | 22.283 | 39.094 | 40.450 | 1.00 31.94 | AAAA |
| ATOM | 736 | C | TYR A | 91 | 25.384 | 34.202 | 38.753 | 1.00 31.56 | AAAA |
| | | õ | | 91 | 26.075 | 35.105 | 39.233 | 1.00 31.21 | AAAA |
| MOTA | 737 | | TYR A | | | | | | |
| ATOM | 738 | N | GLU A | 92 | 24.925 | 33.158 | 39.438 | 1.00 31.51 | AAAA |
| MOTA | 739 | CA | GLU A | 92 | 25.143 | 32.941 | 40.865 | 1.00 32.70 | AAAA |
| | 740 | CB | GLU A | 92 | 24.463 | 31.626 | 41.268 | 1.00 33.55 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 741 | CG | GLU A | 92 | 24.174 | 31.495 | 42.747 | 1.00 34.16 | AAAA |
| ATOM | 742 | CD | GLU A | 92 | 23.311 | 30.278 | 43.087 | 1.00 35.31 | AAAA |
| | 743 | | GLU A | 92 | 23.857 | 29.148 | 43.152 | 1.00 34.30 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 744 | OE2 | GLU A | 92 | . 22.076 | 30.466 | 43.275 | 1.00 35.36 | AAAA |
| MOTA | 745 | С | GLU A | 92 | 26.619 | 32.902 | 41.248 | 1.00 33.02 | AAAA |
| | 746 | ō | GLU A | 92 | 27.073 | 33.623 | 42.140 | 1.00 32.91 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 747 | N | asn a | 93 | 27.358 | 32.049 | 40.550 | 1.00 32.84 | AAAA |
| MOTA | 748 | CA | ASN A | 93 | 28.785 | 31.861 | 40.777 | 1.00 31.92 | AAAA |
| | 749 | CB | ASN A | 93 | 29.015 | 30.437 | 41.278 | 1.00 31.18 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 750 | CG | ASN A | 93 | 27.948 | 29.994 | 42.259 | 1.00 30.34 | AAAA |
| ATOM | 751 | OD1 | ASN A | 93 | 27.723 | 30.642 | 43.271 | 1.00 31.20 | AAAA |
| ATOM | 752 | ND2 | ASN A | 93 | 27.284 | 28.892 | 41.955 | 1.00 29.02 | AAAA |
| | | | | | 29.442 | | 39.411 | 1.00 30.84 | AAAA |
| MOTA | 753 | C | asn a | 93 | | 32.052 | | | |
| MOTA | 754 | 0 | ASN A | 93 | 29.823 | 31.082 | 38.758 | 1.00 30.82 | AAAA |
| ATOM | 755 | N | PRO A | 94 | 29.605 | 33.309 | 38.975 | 1.00 29.56 | AAAA |
| | | | | 94 | 29.312 | 34.590 | 39.626 | 1.00 29.03 | AAAA |
| MOTA | 756 | CD | PRO A | | | | | | |
| ATOM | 757 | CY | PRO A | 94 | 30.209 | 33.564 | 37.671 | 1.00 28.89 | AAAA |
| MOTA | 758 | CB | PRO A | 94 | 29.890 | 35.045 | 37.416 | 1.00 28.22 | AAAA |
| | 759 | CG | PRO A | 94 | 28.839 | 35.377 | 38.435 | 1.00 29.50 | AAAA |
| MOTA | | | | | | | 37.664 | 1.00 28.25 | AAAA |
| MOTA | . 760 | С | PRO A | 94 | . 31.698 | 33.351 | | | |
| ATOM | 761 | Ω | PRO A | 94 | 32.308 | 32.996 | 38.671 | 1.00 28.21 | AAAA |
| ATOM | 762 | N | VAL A | 95 | 32.257 | 33.593 | 36.488 | 1.00 27.36 | AAAA |
| | | | | | 33.676 | 33.530 | 36.247 | 1.00 26.24 | AAAA |
| MOTA | 763 | CA | VAL A | 95 | | | | | |
| MOTA | 764 | C3 | VAL A | 95 | 33.945 | 33.289 | 34.741 | 1.00 26.10 | AAAA |
| ATOM | 765 | CG1 | VAL A | 95 | 35.373 | 33.717 | 34.357 | 1.00 25.47 | AAAA |
| | | | VAL A | 95 | 33.736 | 31.826 | 34.434 | 1.00 25.59 | AAAA |
| ATOM | 766 | | | | | | | | |
| MOTA | 767 | C | VAL A | 95 | 34.178 | 34.919 | 36.647 | 1.00 26.56 | AAAA |
| ATOM | 768 | 0 | VAL A | 95 | 33.560 | 35.937 | 36.3 07 | 1.00 27.18 | AAAA |
| | 769 | N | SER A | 96 | 35.280 | 34.966 | 37.382 | 1.00 25.23 | AAAA |
| MOTA | | | | | | | 37.790 | 1.00 24.51 | AAAA |
| ATOM | 770 | CA | SER A | 96 | 35.858 | 36.237 | | | |
| ATOM | 771 | CЭ | SER A | 96 | 34.935 | 36.961 | 38.774 | 1.00 23.22 | ·AAAA |
| ATOM | 772 | OG | SER A | 96 | 34.941 | 36.297 | 40.014 | 1.00 19.76 | AAAA |
| | | | | | 37.169 | 35.920 | 38.485 | 1.00 24.84 | AAAA |
| ATOM | 773 | C | SER A | 96 | | | | | |
| MOTA | 774 | 0 | SER A | 96 | 37.590 | 34.764 | 38.530 | 1.00 25.97 | AAAA |
| ATOM | 775 | N | TYR A | 97 | 37.824 | 36.933 | 39.03 0 | 1.00 24.02 | AAAA |
| | 776 | CA | TYR A | 97 | 39.047 | 36.664 | 39.744 | 1.00 24.55 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 777 | CB | TYR A | 97 | 40.071 | 37.762 | 39.504 | 1.00 23.94 | AAAA |
| MOTA | 778 | CG | TYR A | 97 | 40.682 | 37.636 | 38.128 | 1.00 23.72 | AAAA |
| | 779 | | TYR A | 97 | 40.177 | 38.341 | 37.039 | 1.00 23.11 | AAAA |
| MOTA | | | | | | | 35.758 | 1.00 23.50 | AAAA |
| MOTA | 780 | CEI | TYR A | 97 | 40.700 | 38.136 | | | |
| MOTA | 781 | CD2 | TYR A | 97 | 41.717 | 36.735 | 37.903 | 1.00 22.25 | AAAA |
| | 782 | | TYR A | 97 | 42.236 | 36.526 | 36.640 | 1.00 22.86 | AAAA |
| ATOM | | | | | 41.730 | 37.217 | 35.572 | 1.00 23.56 | AAAA |
| ATOM | 783 | CZ | TYR A | 97 | | | | | |
| ATOM | 784 | OH | TYR A | 97 | 42.232 | 36.941 | 34.318 | 1.00 24.06 | AAAA |
| | 785 | C | TYR A | 97 | 38.800 | 36.436 | 41.228 | 1.00 25.08 | AAAA |
| MOTA | | | | | | 36.266 | 42.009 | 1.00 26.91 | AAAA |
| MOTA | 786 | 0 | TYR A | 97 | 39.739 | | | | |
| ATOM | 787 | N | ALA A | 98 | 37.522 | 36.406 | 41.589 | 1.00 24.73 | AAAA |
| ATOM | 788 | CA | ALA A | 98 | 37.083 | 36.159 | 42.951 | 1.00 24.50 | aaaa |
| | | | ALA A | | 35.800 | 36.925 | 43.235 | 1.00 24.48 | AAAA |
| ATOM | 789 | C3 | | 98 | | | | | |
| ATOM | 790 | С | ALA A | 98 | 36.824 | 34.661 | 43.088 | 1.00 23.95 | AAAA |
| ATOM | 791 | ο. | ALA A | 98 | 36.929 | 34.100 | 44.171 | 1.00 24.21 | AAAA |
| | | N | MET A | 99 | 36.502 | 34.011 | 41.976 | 1.00 23.10 | AAAA |
| ATCM | 792 | 7.4 | WET W | 33 | 30.302 | 33.011 | | 2.00 20.20 | · · · |
| • | | | | | | | | | • |

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| ATOM | 793 CA MET A | 0.0 | 36 200 | 22 504 | 40 000 | | |
|--------|-----------------|-------|--------|--------|--------|------------|--------|
| | | | 36.208 | 32.584 | | 1.00 22.61 | AAAA |
| MOTA | 794 CB MET A | . 99 | 35.855 | 32.089 | 40.597 | 1.00 23.25 | · AAAA |
| ATOM | 795 CG MET A | 99 | 37.009 | | | | |
| ATOM | | | | 32.003 | 33.007 | | AAAA |
| | | | 36.360 | 31.808 | 37.952 | 1.00 25.21 | AAAA |
| ATOM | 797 CE MET A | . 99 | 35.328 | 30.374 | 38.258 | 1.00 22.04 | AAAA |
| ATOM | 798 C MET A | . 99 | 37.319 | 31.720 | | | |
| MOTA | | | | | | | AAAA |
| | | | 37.052 | 30.695 | 43.199 | 1.00 21.29 | AAAA |
| ATOM | 800 N PHE A | . 100 | 38.567 | 32.111 | 42.380 | 1.00 21.87 | AAAA |
| ATOM | 801 CA PHE A | 100 | 39.650 | 31.322 | | | |
| | | | | | | 1.00 21.11 | AAAA |
| ATOM | 802 CB PHE A | | 40.388 | 30.552 | 41.841 | 1.00 20.25 | AAAA |
| ATOM | 803 CG PHE A | 100 . | 41.451 | 29.648 | 42.375 | 1.00 20.14 | AAAA |
| ATOM | 804 CD1 PHE A | 100 | 41.114 | 28.462 | | | |
| ATOM | | | | | | 1.00 20.49 | AAAA |
| | | | 42.785 | 30.050 | 42.373 | 1.00 19.82 | AAAA |
| MOTA | 806 CE1 PHE A | 100 | 42.090 | 27.695 | 43.646 | 1.00 19.54 | AAAA |
| ATOM | 807 CE2 PHE A | 100 | 43.755 | 29.300 | • | | |
| ATOM | | | | | | 1.00 19.22 | AAAA |
| | | | 43.410 | 28.122 | 43.641 | 1.00 19.47 | AAAA |
| MOTA | 809 C PHE A | 100 | 40.649 | 32.161 | 43.743 | 1.00 21.37 | AAAA |
| MOTA | 810 O PHE A | 100 | 40.959 | 31.822 | 44.887 | 1.00 21.26 | |
| ATOM | | | | | | | AAAA |
| | | | 41.142 | 33.252 | 43.161 | 1.00 20.94 | AAAA |
| ATOM | 812 CA THR A | 101 | 42.119 | 34.097 | 43.847 | 1.00 21.95 | AAAA |
| ATOM | 813 CB THR A | 101 | 42.691 | 35.181 | 42.905 | 1.00 22.21 | |
| ATOM | 814 OG1 THR A | | | | | | AAAA |
| | | | 43.511 | 34.552 | 41.917 | 1.00 22.90 | AAAA |
| ATOM | 815 CG2 THR A | 101 | 43.535 | 36.186 | 43.667 | 1.00 21.38 | AAAA |
| MOTA | 816 C THR A | 101 | 41.584 | 34.755 | 45.117 | 1.00 22.60 | |
| ATOM | 817 O THR A | | 42.248 | | | | |
| | | | | 34.723 | 46.147 | 1.00 23.38 | AAAA |
| MOTA | 818 N GLY A | | 40.394 | 35.343 | 45.049 | 1.00 22.13 | AAAA |
| ATOM | 819 CA GLY A | 102 | 39.826 | 35.972 | 46.227 | 1.00 22.03 | AAAA |
| MOTA | 820 C GLY A | 102 | 39.340 | 34.928 | 47.221 | 1.00 21.36 | |
| ATOM | 821 O GLY A | | | | | | AAAA |
| | | | 39.433 | 35.104 | 48.439 | 1.00 20.02 | AAAA |
| MOTA | 822 N SERA | 103 | 38.816 | 33.833 | 46.677 | 1.00 21.86 | AAAA |
| ATOM | 823 CA SER A | 103 | 38.311 | 32.719 | 47.466 | 1.00 21.68 | AAAA |
| MOTA | 824 CB SER A | | 37.699 | | | | |
| | | • | | 31.668 | 46.557 | 1.00 21.56 | AAAA |
| MOTA | 825 OG SER A | 103 | 36.604 | 32.216 | 45.857 | 1.00 23.67 | AAAA |
| ATOM | 826 C SER A | 103 | 39.450 | 32.098 | 48.229 | 1.00 22.67 | AAAA |
| ATOM | 827 O SER A | 103 | 39.314 | 31.806 | 49.412 | 1.00 22.44 | |
| ATOM | 828 N SER A | | | | | | AAAA |
| | | | 40.578 | 31.898 | 47.545 | 1.00 23.37 | AAAA |
| ATOM | 829 CA SER A | | 41.746 | 31.305 | 48.183 | 1.00 23.50 | AAAA |
| ATOM | 830 CB SER A | 104 | 42.862 | 31.070 | 47.172 | 1.00 24.80 | AAAA |
| ATOM | 831 OG SER A | 104 | 42.441 | 30.169 | 46.175 | 1.00 28.38 | |
| ATOM | 832 C SER A | | | | | | AAAA |
| | | | 42.254 | 32.230 | 49.256 | 1.00 22.79 | AAAA |
| ATOM | 833 O SER A | | 42.707 | 31.794 | 50.307 | 1.00 22.66 | AAAA |
| ATOM | 834 N LEU A | 105 | 42.160 | 33.518 | 48.970 | 1.00 22.08 | AAAA |
| MOTA | 835 CA LEÚ A | | 42.626 | 34.541 | 49.870 | 1.00 21.70 | |
| ATOM | | | | | | | AAAA |
| | | | 42.524 | 35.882 | 49.159 | 1.00 21.89 | AAAA |
| ATOM | 837 CG LEU A | 105 · | 43.332 | 37.038 | 49.718 | 1.00 23.64 | AAAA |
| MOTA | 838 CD1 LEU A | 105 | 44.830 | 36.692 | 49.639 | 1.00 22.01 | AAAA |
| ATOM | 839 CD2 LEU A | | 43.004 | _ | | | |
| | | | | 38.304 | | 1.00 23.60 | AAAA |
| ATOM | 840 C LEUA | | 41.767 | 34.525 | 51.131 | 1.00 22.29 | AAAA |
| MOTA | 841 O LEUA: | 105 | 42.277 | 34.595 | 52.249 | 1.00 21.95 | AAAA |
| ATOM | 842 N ALA A | 106 | 40.458 | 34.429 | 50.934 | 1.00 22.23 | |
| ATOM | 843 CA ALA A | | 39.515 | | | | AAAA |
| | | | | | 52.042 | 1.00 22.32 | AAAA |
| ATOM | 844 CB ALA A | 106 | 38.068 | 34.472 | 51.526 | 1.00 22.05 | AAAA |
| ATOM | 845 C ALA A | 106 | 39.704 | 33.126 | 52.840 | 1.00 21.99 | AAAA |
| ATOM | 846 O ALA A | | 39.578 | | | | |
| | | | | 33.145 | 54.061 | 1.00 23.18 | AAAA |
| ATOM | 847 N THR A 1 | | 40.011 | 32.032 | 52.144 | 1.00 21.24 | AAAA |
| MOTA | 848 CA THRAI | .07 | 40.209 | 30.732 | 52.779 | 1.00 20.60 | AAAA |
| ATOM | 849 CB THR A 1 | | 40.170 | 29.571 | 51.749 | 1.00 19.82 | |
| | | | | | | | AAAA |
| MOTA | | | 38.903 | 29.553 | 51.083 | 1.00 18.56 | AAAA |
| ATOM | 851 CG2 THR A 1 | .07 | 40.360 | 28.242 | 52.455 | 1.00 18.58 | AAAA |
| ATOM | 852 C THR A 1 | .07. | 41.516 | 30.630 | 53.561 | 1.00 21.41 | AAAA |
| ATOM | 853 O THR A 1 | | 41.537 | | | | |
| | | | | 30.040 | 54.646 | 1.00 23.16 | AAAA |
| ATOM | 854 N GLY A 1 | | 42.601 | 31.176 | 53.003 | 1.00 20.14 | AAAA |
| ATOM | 855 CA GLY A 1 | 08 | 43.878 | 31.145 | 53.684 | 1.00 18.20 | AAAA |
| ATOM . | 856 C GLY A 1 | | 43.739 | 31.933 | 54.972 | 1.00 18.43 | |
| | | | | | | | AAAA |
| ATOM | 857 O GLY A 1 | | | 31.600 | 55.998 | 1.00 17.52 | AAAA |
| ATOM | 858 N SER A 1 | U9 | 42.909 | 32.969 | 54.929 | 1.00 18.56 | AAAA |
| | | | | - | | | |

| ATOM | 859 | CA | SER A | 109 | 42.683 | 33.805 | 56.098 | 1.00 19.67 | AAAA |
|--------|-----|-----|-------|-------|--------|--------|-----------------|------------|--------|
| | 860 | CB | SER A | | 41.899 | 35.058 | 55.70 7 | 1.00 20.27 | AAAA |
| ATOM | | | | | | 35.803 | 54.746 | 1.00 21.80 | AAAA |
| MOTA | 861 | OG | SER A | | 42.618 | | | | |
| MOTA | 862 | С | SER A | . 109 | 41.955 | 33.066 | 57.219 | 1.00 19.61 | AAAA |
| ATOM | 863 | 0 | SER A | 109 | 42.078 | 33.426 | 58.388 | 1.00 18.40 | AAAA |
| | | | THR A | | 41.186 | 32.042 | 56.866 | 1.00 19.88 | AAAA |
| ATOM - | 864 | N | | | | | | 1.00 20.51 | AAAA |
| MOTA | 865 | CA | THR A | . 110 | 40.493 | 31.288 | 57.891 | | |
| ATOM | 866 | CB | THR A | 110 | 39.365 | 30.438 | 57.304 | 1.00 20.62 | AAAA |
| | 867 | | THR A | 110 | 38.236 | 31.284 | 57.050 | 1.00 20.80 | AAAA |
| MOTA | | | | | | | 58.262 | 1.00 20.53 | AAAA |
| MOTA | 868 | CG2 | | | 38.974 | 29.313 | | | • |
| ATOM | 869 | С | THR A | 110 | 41.504 | 30.420 | 58.601 | 1.00 20.36 | AAAA |
| | 870 | 0 | THR A | | 41.455 | 30.268 | 59.822 | 1.00 20.78 | AAAA |
| ATOM | | | | | 42.431 | 29.855 | 57.832 | 1.00 20.85 | AAAA |
| ATOM | 871 | N | VAL A | | | | | | |
| ATOM | 872 | CA | VAL A | 111 | 43.480 | 29.053 | 58.423 | 1.00 21.03 | AAAA |
| ATOM | 873 | CB | VAL A | 111 | 44.318 | 28.323 | 57.345 | 1.00 21.05 | AAAA |
| | 874 | | VAL A | | 45.537 | 27.644 | 57.983 | 1.00 19.91 | -AAAA |
| MOTA | | | | | | | 56.648 | 1.00 18.39 | AAAA |
| MOTA | 875 | CGZ | VAL A | 111 | 43.460 | 27.281 | | | |
| ATOM | 876 | С | VAL A | 111 | 44.374 | 30.005 | 59.232 | 1.00 21.84 | AAAA |
| ATOM | 877 | 0 | VAL A | 111 | 44.825 | 29.671 | 60.331 | 1.00 22.73 | · AAAA |
| | | | | | 44.612 | 31.204 | | 1.00 21.62 | AAAA |
| ATOM | 878 | N | GLN A | | | | | | |
| ATOM | 879 | CA | GLN A | 112 | 45.449 | 32.133 | 59.452 | 1.00 21.89 | AAAA |
| ATOM | 880 | CB | GLN A | 112 | 45.630 | 33.450 | 58.690 | 1.00 22.50 | AAAA |
| | | CG | GLN A | | 46.288 | 33.283 | 57.335 | 1.00 23.68 | AAAA |
| ATOM | 881 | | | | | | 5 6 .569 | 1.00 23.18 | AAAA |
| ATOM | 882 | CD | GLN A | | 46.414 | 34.578 | | | |
| MOTA | 883 | OE1 | GLN A | . 112 | 47.389 | 35.310 | 56.722 | 1.00 23.86 | AAAA |
| ATOM | 884 | NE2 | GLN A | 112 | 45.413 | 34.879 | 55.752 | 1.00 21.90 | AAAA |
| | | C | GLN A | | 44.766 | 32.383 | 60.774 | 1.00 21.84 | AAAA |
| ATCM | 885 | | - | | | | 61.835 | 1.00 22.47 | AAAA |
| ATOM | 886 | 0 | GLN A | | 45.389 | 32.316 | | | |
| MOTA | 887 | N | ALA A | 113 | 43.468 | 32.651 | 60.700 | 1.00 21.34 | AAAA |
| ATOM | 888 | CA | ALA A | 113 | 42.682 | 32.934 | 61.884 | 1.00 20.84 | AAAA |
| | | | | | 41.244 | | 61.504 | 1.00 18.52 | AAAA |
| MOTA | 889 | CB | ALA A | | | | | 1.00 21.75 | AAAA |
| ATOM | 890 | C | ALA A | 113 | 42.795 | 31.782 | 62.865 | | |
| MOTA | 891 | 0 | ALA A | 113 | 42.880 | 31.985 | 64.084 | 1.00 22.24 | AAAA |
| | 892 | N | ILE A | | 42.797 | 30.569 | 62.329 | 1.00 22.54 | AAAA |
| ATOM | | | | | 42.891 | 29.393 | 63.160 | 1.00 23.16 | AAAA |
| MOTA | 893 | | ILE A | | | | 62.352 | 1.00 23.33 | AAAA |
| ATOM | 894 | CB | ILE A | 114 | 42.557 | 28.146 | | | |
| ATOM | 895 | CG2 | ILE A | 114 | 42.939 | 26.912 | 63.106 | 1.00 23.80 | AAAA |
| | 896 | CG1 | ILE A | 114 | 41.058 | 28.130 | 62.047 | 1.00 23.48 | AAAA |
| MOTA | | | ILE A | | 40.610 | 26.951 | 61.204 | 1.00 22.08 | AAAA |
| MOTA | 897 | | | | | | 63.792 | 1.00 24.33 | AAAA |
| ATOM | 898 | С | ILE A | 114 | 44.268 | 29.270 | | | |
| ATOM | 899 | 0 | ILE A | 114 | 44.373 | 29.013 | 64.990 | 1.00 25.30 | AAAA |
| | 900 | N | GLU A | 115 | 45.319 | 29.490 | 63.002 | 1.00 24.96 | AAAA |
| ATOM | | | | | 46.699 | 29.395 | 63.503 | 1.00 26.61 | AAAA |
| MOTA | 901 | CA | GLU A | | | | 62.406 | 1.00 24.75 | AAAA |
| ATOM | 902 | CB | GLU A | 115 | 47.708 | 29.753 | | | |
| ATOM | 903 | CG | GLU A | 115 | 47.444 | 29.033 | 61.103 | 1.00 25.80 | AAAA |
| | 904 | CD | GLU A | 115 | 48.471 | 29.323 | 60.030 | 1.00 26.07 | AAAA |
| MOTA | | | | | 48.911 | 30.484 | 59.940 | 1.00 27.15 | AAAA |
| ATOM | 905 | | GLU A | | | | 59.260 | 1.00 25.45 | AAAA |
| ATOM | 906 | OE2 | GLU A | | 48.819 | 28.402 | | | |
| ATOM | 907 | С | GLU A | 115 | 46.877 | 30.340 | 64.680 | 1.00 27.89 | AAAA |
| | 908 | 0 | GLU A | 115 | 47.480 | 29.975 | 65.695 | 1.00 28.04 | AAAA |
| ATOM | | | | | 46.337 | 31.552 | 64.531 | 1.00 29.15 | AAAA |
| ATOM | 909 | N | GLU A | 110 | | | 65.563 | 1.00 29.42 | AAAA |
| MOTA | 910 | CA | GLU A | | 46.408 | 32.579 | | | |
| ATOM | 911 | CB | GLU A | 116 | 45.751 | 33.871 | 65.082 | 1.00 28.26 | AAAA |
| | 912 | CG | GLU A | | 46.482 | 34.529 | 63.945 | 1.00 28.93 | AAAA |
| ATOM | | | | | | 34.937 | 64.318 | 1.00 28.32 | AAAA |
| MOTA | 913 | CD | GLU A | | 47.902 | | | 1.00 27.68 | AAAA |
| ATOM | 914 | | GLU A | | 48.081 | 35.878 | 65.123 | | |
| ATOM | 915 | OE2 | GLU A | 116 | 48.838 | 34.297 | 63.810 | 1.00 27.38 | AAAA |
| | 916 | c | GLU A | | 45.737 | 32.126 | 66.845 | 1.00 29.77 | AAAA |
| ATOM | | | | | 46.338 | 32.196 | 67.920 | 1.00 30.29 | AAAA |
| ATOM | 917 | 0 | GLU A | | | | | 1.00 29.64 | |
| ATCM | 918 | N | PHE A | . 117 | 44.492 | 31.665 | 66.727 | | |
| | 919 | CA | PHE A | 117 | 43.741 | 31.204 | 67.887 | 1.00 29.33 | AAAA |
| ATOM | | | PHE A | | 42.425 | 30.552 | 67.480 | 1.00 28.89 | AAAA |
| Mota | 920 | CB | | | | | 68.651 | 1.00 28.93 | AAAA |
| ATCM | 921 | CG | PHE A | | 41.604 | 30.087 | | | |
| ATOM | 922 | CD1 | PHE A | 117 | 41.010 | 31.010 | 69.510 | 1.00 28.42 | AAAA |
| | 923 | | PHE A | | 41.441 | 28.723 | 68.910 | 1.00 29.06 | AAAA |
| ATCM | - | | | | 40.261 | 30.588 | 70.610 | 1.00 28.68 | AAAA |
| ATOM | 924 | CEL | PHE A | 111 | 40.201 | 50.500 | | | |
| | | | | | - | | | | |

| MOTA | 925 | CE2 | . PHE | A 117 | 40.695 | 28.284 | 70.009 | 1.00 29.16 | AAAA |
|--------|-------|------|-------|-------|--------|--------|--------|------------|-------|
| ATOM | 926 | CZ | PHE | A 117 | 40.103 | 29.227 | 70.862 | 1.00 29.03 | AAAA |
| ATOM | 927 | C | PHE | A 117 | 44.545 | 30.195 | 68.671 | 1.00 29.22 | AAAA |
| MOTA | 928 | 0 | PHE | A 117 | 44.677 | 30.315 | 69.884 | 1.00 30.29 | AAAA |
| ATOM | 929 | N | LEU | A 118 | 45.066 | 29.195 | 67.965 | 1.00 29.24 | AAAA |
| ATOM | 930 | CA | LEU | A 118 | 45.864 | 28.145 | 68.576 | 1.00 29.50 | AAAA |
| MOTA | 931 | CB | LEU | A 118 | 46.182 | 27.047 | 67.550 | 1.00 28.57 | AAAA |
| ATOM | 932 | CG | LEU | A 118 | 44.962 | 26.296 | 66.989 | 1.00 28.16 | AAAA |
| ATOM | 933 | CD1 | LEU | A 118 | 45.421 | 25.090 | 66.191 | 1.00 25.58 | AAAA |
| MOTA | 934 | CD2 | LEU | A 118 | 44.053 | 25.846 | 68.128 | 1.00 27.64 | AAAA |
| ATOM | 935 | С | LEU | A 118 | 47.150 | 28.649 | 69.227 | 1.00 30.14 | AAAA |
| ATOM | 936 | 0 | LEU . | A 118 | 47.727 | 27.954 | 70.056 | 1.00 29.94 | AAAA |
| ATOM | 937 | N | LYS | A 119 | 47.602 | 29.845 | 68.847 | 1.00 31.36 | AAAA |
| ATOM | 938 | CA | LYS . | A 119 | 48.798 | 30.451 | 69.448 | 1.00 32.52 | AAAA |
| ATOM | 939 | CB | LYS . | A 119 | 49.396 | 31.539 | 68.559 | 1.00 32.38 | AAAA |
| ATOM | 940 | CG | LYS . | A 119 | 49.882 | 31.108 | 67.199 | 1.00 33.03 | AAAA |
| ATOM | 941 | CD | | A 119 | 50.371 | 32.321 | 66.411 | 1.00 32.74 | AAAA |
| ATOM | 942 | CE | | A 119 | 50.681 | 31.939 | 64.972 | 1.00 33.94 | AAAA |
| ATOM | 943 | NZ | | A 119 | 51.125 | 33:099 | 64,152 | 1.00 34.93 | AAAA |
| ATOM | 944 | С | | A 119 | 48.385 | 31.143 | 70.744 | 1.00 33.74 | AAAA |
| ATOM | 945 | Ō | | A 119 | 49.218 | 31.748 | 71.413 | 1.00 34.85 | AAAA |
| ATOM | 946 | N | | A 120 | 47.096 | 31.079 | 71.073 | 1.00 33.68 | AAAA |
| MOTA | 947 | CA | | A 120 | 46.600 | 31.736 | 72.263 | 1.00 33.69 | AAAA |
| ATOM | 948 | C | | A 120 | 45.987 | 33.110 | 71.988 | 1.00 34.11 | AAAA |
| ATOM | 949 | ō | | A 120 | 45.588 | 33.802 | 72.932 | 1.00 33.65 | AAAA |
| ATOM | 950 | N | | A 121 | 45.904 | 33.513 | 70.717 | 1.00 33.58 | AAAA |
| ATOM | 951 | CA | | A 121 | 45.326 | 34.820 | 70.368 | 1.00 33.35 | AAAA |
| ATOM | 952 | CB | | A 121 | 46.194 | 35.537 | 69.341 | 1.00 33.18 | AAAA |
| ATOM | 953 | CG | | A 121 | 47.570 | 35.828 | 69.859 | 1.00 34.31 | AAAA |
| ATOM | 954 | | ASN A | | 48.333 | 34.921 | 70.154 | 1.00 35.67 | AAAA |
| ATOM | 955 | | ASN A | | 47.897 | 37.096 | 69.975 | 1.00 34.18 | AAAA |
| MOTA | 956 | С | | A 121 | 43.888 | 34.805 | 69.839 | 1.00 32.85 | AAAA |
| ATOM | 957 | 0 | | A 121 | 43.304 | 33.751 | 69.599 | 1.00 32.78 | AAAA |
| ATOM | 958 | N | | A 122 | 43.338 | 36.003 | 69.655 | 1.00 32.47 | AAAA |
| ATOM | 959 | CA | | A 122 | 41.980 | 36.200 | 69.148 | 1.00 30.89 | AAAA |
| ATOM | 960 | CB | | A 122 | 41.182 | 37.145 | 70.070 | 1.00 31.05 | AAAA |
| ATOM | 961 | CG1 | VAL A | A 122 | 39.831 | 37.423 | 69.489 | 1.00 30.95 | AAAA: |
| ATOM | 962 | CG2 | VAL A | 122 | 41.038 | 36.516 | 71.440 | 1.00 31.19 | AAAA |
| ATOM | 963 | С | VAL 3 | 122 | 42.056 | 36.805 | 67.750 | 1.00 30.19 | AAAA |
| ATOM . | 964 | 0 | VAL A | 122 | 42.694 | 37.840 | 67.535 | 1.00 31.28 | AAAA |
| ATOM | 965 | N | ALA A | 123 | 41.405 | 36.147 | 66.800 | 1.00 28.62 | AAAA |
| ATOM | 966 | CA | ALA A | 123 | 41.415 | 36.589 | 65.421 | 1.00 26.49 | AAAA |
| ATOM | 967 | CB | ALA A | 1/123 | 42.323 | 35.708 | 64.599 | 1.00 26.51 | AAAA |
| ATOM | 968 | С | ALA A | 123 | 40.038 | 36.570 | 64.836 | 1.00 25.59 | AAAA |
| ATOM | 969 | 0 | ALA A | 123 | 39.173 | 35.814 | 65.252 | 1.00 26.27 | AAAA |
| ATOM | 970 | N | PHE A | 124 | 39.848 | 37.421 | 62.847 | 1.00 25.44 | AAAA |
| ATOM | 971 | CA | PHE A | 124 | 38.590 | 37.534 | 61.156 | 1.00 23.87 | AAAA |
| ATOM | 972 | CB | PHE A | 124 | 37.832 | 38.779 | 63.646 | 1.00 23.58 | AAAA |
| MOTA | 973 | CG . | PHE A | 124 | 36.591 | 39.119 | 62.841 | 1.00 23.71 | AAAA |
| ATOM. | 974 | CD1 | PHE A | 124 | 35.668 | 38.140 | 62.495 | 1.00 23.44 | AAAA |
| ATOM | 975 | CD2 | PHE A | 124 | 36.311 | 40.449 | 62.498 | 1.00 23.75 | AAAA |
| ATOM | 976 | CE1 | PHE A | 124 | 34.479 | 38.483 | 61.823 | 1.00 23.31 | AAAA |
| MOTA | 977 | CE2 | PHE A | 124 | 35.131 | 40.796 | 61.833 | 1.00 21.71 | AAAA |
| | . 978 | | PHE A | | 34.217 | 39.815 | 61.497 | 1.00 22.35 | AAAA |
| MOTA | 979 | C . | PHE A | 124 | 38.951 | 37.673 | 61.700 | 1.00 23.26 | AAAA |
| ATOM | 980 | 0 | PHE A | 124 | 39.720 | 38.555 | 61.323 | 1.00 22.29 | AAAA |
| ATOM | 98,1 | N : | ASN A | 125 | 38.427 | 36.759 | 60.897 | 1.00 23.24 | AAAA |
| ATOM | 962 | CA Z | ASN A | 125 | 38.622 | 36.785 | 59.457 | 1.00 21.08 | AAAA |
| ATOM | 983 | CB 2 | ASN A | 125 | 39.181 | 35.470 | 58.951 | 1.00 19.90 | AAAA |
| ATOM | 984 | | ASN A | | 39.098 | 35.360 | 57.454 | 1.00 20.64 | AAAA |
| ATOM | 285 | | ASN A | 125 | 39.389 | 36.317 | 56.748 | 1.00 21.63 | AAAA |
| ATOM | 986 | | ASN A | | 38.721 | 34.190 | 56.956 | 1.00 19.93 | AAAA |
| ATOM | 987 | | ASN A | | 37.269 | 37.059 | 58.813 | 1.00 20.19 | AAAA |
| ATOM | 988 | | ASN A | | 36.469 | 36.148 | 58.579 | 1.00 19.21 | AAAA |
| MOTA | 989 | N I | PRO A | 126 | 36.991 | 38.340 | 58.543 | 1.00 19.14 | AAAA |
| ATOM | 990 | CD I | PRO A | 126 | 37.893 | 39.460 | 58.858 | 1.00 19.22 | AAAA |
| • | | | | | | - | _ | | |

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| ATOM | 991 | CA | PRO A | 126 | 35.766 | 38.849 | 57,932 | 1 00 | 19.52 | 2222 |
|------|------|-----|---------|-------|--------|--------|--------|------|--------|-------------|
| ATOM | 992 | СВ | PRO A | | 36.005 | 40.359 | 57.941 | | 18.55 | AAAA |
| ATOM | 993 | CG | PRO A | | 37.511 | 40.465 | 57.799 | | | AAAA |
| MOTA | 994 | c | PRO A | | | | | | 17.97 | AAAA |
| | 995 | Ö | | | 35.456 | 38.313 | 56.526 | | 19.41 | AAAA |
| ATOM | • | | PRO A | | 34.303 | 38.349 | 56.080 | | 19.68 | AAAA |
| MOTA | 996 | N | ALA A | | 36.477 | 37.814 | 55.835 | | 18.17 | AAAA |
| MOTA | 997 | CA | ALA A | | 36.283 | 37.314 | 54.481 | | 17.66 | AAAA |
| ATOM | 998 | CB | ALA A | | 37.547 | 37.520 | 53.658 | | 17.08 | AAAA |
| MOTA | 999 | С | ALA A | | 35.875 | 35.857 | 54.443 | 1.00 | 17.46 | AAAA |
| ATOM | 1000 | 0 | ALA A | . 127 | 35.438 | 35.359 | 53.409 | 1.00 | 18.92 | AAAA |
| ATOM | 1001 | N | GLY A | . 128 | 36.019 | 35.180 | 55.570 | 1.00 | 15.94 | AAAA |
| MOTA | 1002 | CA | GLY A | . 128 | 35.685 | 33.780 | 55.642 | 1.00 | 15.45 | AAAA |
| MOTA | 1003 | С | GLY A | . 128 | 34.226 | 33.593 | 55.955 | 1.00 | 16.08 | AAAA |
| ATOM | 1004 | 0 | GLY A | 128 | 33.485 | 34.557 | 55.997 | 1.00 | 15.43 | AAAA |
| ATOM | 1005 | N | GLY A | 129 | 33.821 | 32.353 | 56.198 | 1.00 | 16.77 | AAAA |
| ATOM | 1006 | CA | GLY A | 129 | 32.426 | 32.082 | 56.462 | | 17.82 | AAAA |
| ATOM | 1007 | C | GLY A | 129 | 31.669 | 31.822 | 55.169 | | 18.64 | AAAA |
| ATOM | 1008 | 0 | GLY A | | 30.469 | 32.051 | 55.108 | | 18.48 | AAAA |
| ATOM | 1009 | N | MET A | | 32.380 | 31.368 | 54.137 | | 20.45 | AAAA |
| MOTA | 1010 | CA | MET A | | 31.790 | 31.029 | 52.826 | | 21.60 | AAAA |
| ATOM | 1011 | CB | MET A | | 32.866 | 31.117 | 51.744 | | 22.02 | AAAA |
| ATOM | 1012 | CG | MET A | | 33.551 | 32.472 | 51.698 | | 21.75 | AAAA |
| ATOM | 1013 | SD | MET A | | 34.971 | 32.567 | 50.599 | | 24.75 | |
| ATOM | 1014 | CE | MET A | | 34.268 | 32.137 | 49.048 | | 24.40 | AAAA |
| ATOM | 1015 | C | MET A | | 31.328 | 29.587 | 53.002 | | 22.08 | AAAA |
| ATOM | 1016 | Õ | MET A | | 31.970 | 28.641 | 52.546 | | 22.98 | AAAA |
| ATOM | 1017 | N | HIS A | | 30.184 | | 53.659 | | | AAAA |
| | 1017 | CA | HIS A | | 29.618 | 29.452 | | | 22.25 | AAAA |
| ATOM | | | | | | 28.171 | 54.062 | | 20.49 | AAAA |
| ATOM | 1019 | CB | HIS A | | 28.832 | 28.421 | 55.342 | | 20.00 | AAAA |
| ATOM | 1020 | CG | HIS A | | 27.679 | 29.360 | 55.161 | | 17.93 | AAAA. |
| ATOM | 1021 | | HIS A | | 27.091 | 29.846 | 54.043 | | 17.88 | AAAA |
| ATOM | 1022 | | HIS A | | 26.952 | 29.854 | 56.219 | | 19.33 | AAAA |
| ATOM | 1023 | | HIS A | | 25.968 | 30.607 | 55.758 | | 16.99 | AAAA |
| ATOM | 1024 | | HIS A | | 26.031 | 30.617 | 54.441 | | 17.43 | AAAA |
| ATOM | 1025 | С | HIS A | | 28.763 | 27.332 | 53.141 | | 19.97 | AAAA |
| ATOM | 1026 | 0 | HIS A | | 28.330 | 26.262 | 53.541 | | 19.61 | AAAA |
| MOTA | 1027 | N | HIS A | | 28.518 | 27.796 | 51.923 | | 20.11 | AAAA |
| ATOM | 1028 | CA | HIS A | | 27.673 | 27.058 | 50.994 | | 17.76 | AAAA |
| ATOM | 1029 | CB | HIS A | | 26.879 | 28.044 | 50.127 | | 16.76 | AAAA |
| ATOM | 1030 | CG | HIS A | | 25.824 | 28.815 | 50.862 | | 15.35 | AAAA |
| ATOM | 1031 | | HIS A | | 25.567 | 30.146 | 50.920 | | 14.15 | AAAA |
| ATOM | 1032 | | HIS A | | 24.804 | 28.200 | 51.557 | | 16.15 | AAAA |
| ATOM | 1033 | | HIS A | | 23.966 | 29.119 | 52.005 | | 14.13 | AAAA |
| MOTA | 1034 | | HIS A | | 24.405 | 30.307 | 51.632 | | 14.65 | AAAA |
| MOTA | 1035 | С | HIS A | | 28.355 | 26.051 | 50.065 | | 17.99 | AAAA |
| ATOM | 1.36 | 0 | HIS A | | 27.742 | 25.053 | 49.684 | | 18.54 | . AAAA |
| MOTA | 1537 | N | ALA A | | 29.604 | 26.305 | 49.690 | | 17.82 | AAAA |
| ATOM | 1638 | CA | ALA A | | 30.300 | 25.441 | 48.742 | | 18.38 | AAAA |
| ATOM | 1039 | CB | ALA A | 133 | 31.684 | 25.961 | 48.507 | 1.00 | 17.53 | AAAA |
| ATOM | 1040 | C | ALA A | 133 | 30.366 | 23.970 | 49.130 | 1.00 | 20.92 | AAAA |
| ATOM | 1041 | 0 | ALA A | 133 | 30.578 | 23.633 | 50.298 | 1.00 | 21.79 | AAAA |
| ATOM | 1042 | И | PHE A | 134 | 30.184 | 23.086 | 48.152 | 1.00 | 20.58 | AAAA |
| ATOM | 1043 | CA | PHE A | 134 | 30.258 | 21.663 | 48.455 | 1.00 | 21.38 | AAAA |
| ATOM | 1044 | CB | PHE A | 134 | 29.168 | 20.860 | 47.731 | 1.00 | 19.41 | AAAA |
| ATOM | 1045 | CG | PHE A | 134 | 27.772 | 21.229 | 48.126 | | 18.32 | AAAA . |
| MOTA | 1046 | CD1 | PHE A | 134 | 27.027 | 22.099 | 47.357 | 1.00 | 19.22 | AAAA |
| MOTA | 1047 | CD2 | PHE A | 134 | 27.193 | 20.701 | 49.271 | | 19.14 | AAAA |
| ATOM | 1048 | | PHE A | | 25.714 | 22.438 | 47.726 | | 18.56 | AAAA |
| ATOM | 1049 | | PHE A | | 25.889 | 21.036 | 49.644 | | 17.72 | AAAA |
| ATOM | 1050 | | PHE A | | 25.158 | 21.903 | 48.866 | | 18.01 | AAAA |
| MOTA | 1051 | | PHE A | | 31.625 | 21.124 | 48.081 | | 22.90 | AAAA |
| ATOM | 1052 | | PHE A | | 32.459 | 21.833 | 47.544 | | 23.37 | AAAA |
| ATOM | 1053 | | LYS A | | 31.842 | 19.861 | 48.390 | | 24.63 | AAAA |
| ATOM | 1054 | | LYS A . | | 33.095 | 19.195 | 48.122 | | 27.16 | AAAA |
| ATOM | 1055 | | LYS A | | 32.926 | 17.714 | 48.480 | | 28.53 | AAAA |
| • | 1056 | | LYS A | | 34.133 | 16.843 | 48.292 | | 31.01 | |
| ATOM | 1030 | ÇG | mra w | | 24.133 | 10.043 | | 1.00 | ~ 1.01 | AAAA |
| | | | | | | | | | | |

| MOTA | 1057 | CD | LYS A | 135 | 33.879 | 15.472 | 48.910 | 1.00 | 32.75 | AAAA |
|------|------|-------------|---------|--------------|-----------------|--------|--------|------|---------------|---|
| | 1050 | CE | | | | | | | | • |
| ATOM | 1058 | CE | LYS A | 122 | 33.961 | 15.495 | 50.457 | 1.00 | 33.96 | AAAA |
| MOTA | 1059 | NZ | LYS A | 135 | 35.371 | 15.664 | 50.976 | 1.00 | 33.04 | AAAA |
| | | | | | | | | | | |
| MOTA | 1060 | С | LYS A | 122 | 33.577 | 19.390 | 46.673 | 1.00 | 27.37 | AAAA |
| ATOM | 1061 | 0 | LYS A | 135 | 34.769 | 19.596 | 46.437 | 1.00 | 27.35 | AAAA |
| | | | | | | | | | | |
| ATOM | 1062 | N | SER A | | 32.658 | 19.354 | 45.714 | 1.00 | 27.32 | AAAA |
| MOTA | 1063 | CA | SER A | 136 | 33.028 | 19.527 | 44.313 | 1 00 | 28.31 | AAAA |
| | | | | | | | | | | |
| MOTA | 1064 | CB | SER A | 136 | 33.093 | 18.162 | 43.626 | 1.00 | 28.56 | AAAA |
| MOTA | 1065 | OG | SER A | 136 | 33.822 | 17.242 | 44.417 | 1 00 | 29.28 | AAAA |
| | | | | | | | | | | |
| MOTA | 1066 | С | SER A | 136 | 31.993 | 20.395 | 43.599 | 1.00 | 28.91 | AAAA |
| MOTA | 1067 | 0 | SER A | 176 | 31.568 | 20.080 | 42.486 | 1 00 | 28.78 | |
| | | | | | | | | | | AAAA |
| ATOM | 1068 | N | ARG A | 137 | 31.595 | 21.502 | 44.212 | 1.00 | 29.08 | .AAAA |
| MOTA | 1069 | CA | ARG A | 137 | 30.574 | 22.311 | 43.576 | 1 00 | 29.66 | |
| - | | | | | | | | | | AAAA |
| MOTA | 1070 | CB | ARG A | 137 | 29.259 | 21.528 | 43.657 | 1.00 | 31.65 | AAAA |
| ATOM | 1071 | CG | ARG A | 127 | 27.989 | 22.273 | 43.355 | 1 00 | 33.8 <i>9</i> | |
| | | | | | | | | | | AAAA |
| ATOM | 1072 | $^{\rm CD}$ | ARG' A | 137 | 26.862 | 21.267 | 43.373 | 1.00 | 35.93 | AAAA |
| | 1073 | NE | | | 26 061 | | 42 220 | - | | |
| MOTA | | | ARG A | | 26.961 | 20.366 | 42.228 | | 36.31 | AAAA |
| ATOM | 1074 | CZ | ARG A | 137 | 26.505 | 20.660 | 41.015 | 1.00 | 35.99 | AAAA |
| | _ | | ARG A | | | | | | | |
| ATOM | 1075 | | | | 25.915 | 21.834 | 40.798 | | 34.63 | AAAA |
| ATOM | 1076 | NH2 | ARG A | 137 | 26.650 | 19.786 | 40.025 | 1.00 | 35.35 | AAAA |
| | | С | | | | | | | | |
| MOTA | 1077 | _ | ARG A | | 30.402 | 23.723 | 44.116 | 1.00 | 28.53 | AAAA |
| ATOM | 1078 | 0 | ARG A | 137 | 30.418 | 23.946 | 45.324 | 1.00 | 28.51 | AAAA |
| | | | | | | | | | | |
| ATOM | 1079 | N | ALA A | | 30.247 | 24.673 | 43.202 | 1.00 | 27.53 | AAAA |
| MOTA | 1080 | CA | ALA A | 138 | 3 0. 039 | 26.063 | 43.581 | 1.00 | 27.64 | AAAA |
| | | | | | | | | | | |
| MOTA | 1081 | CB | ALA A | | 30.236 | 26.984 | 42.381 | | 27.87 | AAAA |
| ATOM | 1082 | С | ALA A | 138 | 28.601 | 26.130 | 44.079 | 1.00 | 27.27 | AAAA |
| | | | | | | | | | | |
| MOTA | 1083 | 0 | ALA A | 130 | 2 7 .769 | 25.321 | 43.671 | 1.00 | 28.30 | AAAA |
| ATOM | 1084 | N | ASN A | 139 | 28.292 | 27.080 | 44.951 | 1.00 | 26.16 | AAAA |
| | | | | | | | | | 25.39 | |
| ATOM | 1085 | CA | ASN A | | 26.945 | 27.134 | 45.480 | | | AAAA |
| ATOM | 1086 | CB | ASN A | 139 | 26.673 | 25.847 | 46.282 | 1.00 | 24.58 | AAAA |
| | | CG | ASN A | | | | | | | |
| MOTA | 1087 | | | | 25.343 | 25.872 | 47.017 | | 25.37 | AAAA |
| ATOM | 1088 | OD1 | ASN A | 139 | 24.272 | 26.017 | 46.413 | 1.00 | 24.20 | AAAA |
| | 1089 | | ASN A | | 25.408 | 25.720 | 48.338 | | 24.91 | AAAA |
| atom | | | | | | | | | | |
| MOTA | 1090 | Ç | ASN A | 139 . | 26.683 | 28.358 | 46.341 | 1.00 | 24.90 | AAAA |
| | 1091 | Ö | ASN A | | 27.346 | 28.570 | 47.348 | | 24.98 | AAAA |
| MOTA | | | | | | | | | • | |
| ATOM | 1092 | N | GLY A | 140 | 25.702 | 29.145 | 45.916 | 1.00 | 24.46 | AAAA |
| | 1093 | CA | GLY A | | 25.294 | 30.336 | 46.625 | | 22.96 | AAAA |
| ATOM | | | | | | | | | | |
| ATOM | 1094 | C | GLY A | 1.40 | 26.383 | 31.358 | 46.755 | 1.00 | 22.24 | AAAA |
| | | Ó | | | | | 47.867 | | | |
| MOTA | 1095 | | GLY A | | 26.663 | 31.817 | | | 23.09 | AAAA |
| ATOM | 1096 | N | PHE A | 141 | 26.992 | 31.711 | 45.625 | 1.00 | 20.60 | AAAA |
| | | CA | | | 28.075 | 32.700 | 45.572 | | 19.43 | |
| MOTA | 1097 | | PHE A | | | | | | | AAAA |
| ATOM | 1098 | CB | PHE A 1 | 141 | 27.758 | 33.920 | 46.430 | 1.00 | 19.86 | AAAA |
| | 1099 | CG | PHE A | 1.4.1 | 26.453 | 34.577 | 46.114 | 3 00 | 21.18 | AAAA |
| MOTA | | | | | | | | | | |
| ATOM | 1100 | CD1 | PHE A 1 | L41 | 25.974 | 35.592 | 46.934 | 1.00 | 20.49 | AAAA |
| | 1101 | CD2 | PHE A I | 1.4.1 | 25.723 | 34.218 | 44.985 | 1 00 | 21.42 | · AAAA |
| MOTA | | | | | | | | | | |
| MOTA | 1102 | CEI | PHE A 1 | 141 | 24.800 | 36.242 | 46.638 | 1.00 | ?2.45 | AAAA |
| ATOM | 1103 | CES | PHE A 1 | 41 | 24.540 | 34.859 | 44.672 | 1.00 | :1.76 | AAAA |
| | | | | | | | | | | |
| ATOM | 1104 | CZ | PHE A 1 | 141 | 24.072 | 35.881 | 45.499 | 1.00 | ^3.05 | AAAA |
| MOTA | 1105 | С | PHE A 1 | 41 | 29.396 | 32.132 | 46.069 | 1 00 | 18.68 | AAAA |
| | | | | | | | | | | |
| MOTA | 1106 | 0 | PHE A 1 | 41 | 30.438 | 32.784 | 45.944 | 1.00 | 19.19 | AAAA |
| ATOM | 1107 | N | CYS A 1 | 42 | 29.367 | 30.930 | 46.635 | 1.00 | 16.93 | AAAA |
| | | | | | | | | | | |
| MOTA | 1108 | CA | CYS A 1 | .42 | 30.594 | 30.332 | 47.150 | 1.00 | 16.80 | AAAA · |
| ATOM | 1109 | CB | CYS A 1 | 42 | 30.323 | 29.689 | 48.509 | 1 00 | 16.51 | AAAA |
| | | | | | | | | | | |
| MOTA | 1110 | SG | CYS A 1 | .42 • • | 29.524 | 30.826 | 49.617 | 1.00 | 15.01 | AAAA |
| | 1111 | С | CYS A 1 | 42 | 31.227 | 29.315 | 46.221 | 1 00 | 16.45 | AAAA |
| MOTA | | | | | | | | | | |
| MOTA | 1112 | 0 | CYS A 1 | 42 | 30.533 | 28.565 | 45.556 | 1.00 | 15.32 | AAAA |
| | 1113 | N | TYR A 1 | 43 | 32.558 | 29.311 | 46.190 | 1.00 | 18.39 | AAAA |
| MOTA | - | | | | | | | | | |
| MOTA | 1114 | CA | TYR A 1 | د <u>4</u> 3 | 33.340 | 28.394 | 45.362 | 1.00 | 18.63 | AAAA |
| ATOM | 1115 | CB | TYR A 1 | | 34.298 | 29.154 | 44.438 | 1 00 | 19.48 | AAAA |
| | | | | | | | | | | |
| MOTA | 1116 | CG | TYR A 1 | 43 | 33.664 | 30.214 | 43.571 | 1.00 | 19.55 | AAAA |
| ATOM | 1117 | | TYR A 1 | | 33.480 | 31.510 | 44.043 | 1 00 | 20.27 | AAAA |
| | | | | | | | | | | |
| ATOM | 1118 | | TYR A 1 | | 32.856 | 32.473 | 43.261 | | 21.63 | AAAA |
| ATOM | 1119 | CD2 | TYR A 1 | 43 | 33.212 | 29.910 | 42.292 | | 20.14 | AAAA |
| | | | | | | | | | | |
| ATOM | 1120 | CE2 | TYR A 1 | 4 S | 32.588 | 30.863 | 41.507 | T.00 | 20.82 | AAAA |
| ATOM | 1121 | CZ | TYR A 1 | 43 | 32.414 | 32.135 | 41.998 | 1.00 | 20.90 | AAAA |
| • | | | | | | | | | | |
| ATOM | 1122 | ОН | TYR A 1 | 47 | 31.787 | 33.071 | 41.228 | 1.00 | 23.36 | AAAA |
| | | | | | | | - | | | • |

| ATOM | 1123 | С | TYR A | 143 | 34.162 | 27.490 | 46.283 | 1.00 19.06 | AAAA |
|---------|------|------|---------|-------|--------|--------|--------|------------|-------------|
| | | | | | | 26.289 | | 1.00 18.40 | AAAA |
| MOTA | 1124 | 0 | TYR A | 143 | 34.319 | | 46.032 | | |
| 7. FDOM | 1125 | N | ILE A | 144 | 34.695 | 28.087 | 47.344 | 1.00 19.15 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 1126 | CA | ILE A | 144 | 35.490 | 27.350 | 48.315 | 1.00 19.97 | AAAA |
| | 1127 | CB | ILE A | 144 | 36.952 | 27.861 | 48.355 | 1.00 19.74 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 1128 | CG2 | ILE A | 144 | 37.757 | 27.088 | 49.410 | 1.00 18.03 | AAAA |
| | | | ILE A | | 37.584 | 27.671 | 46.965 | 1.00 20.12 | AAAA |
| ATOM | 1129 | CGT | TUE W | 144 | | | | | |
| ATOM | 1130 | CD1 | ILE A | 144 | 39.053 | 28.072 | 46.846 | 1.00 21.05 | AAAA |
| | | | | | | | | 1 00 20 22 | AAAA |
| ATOM | 1131 | С | ILE A | 144 | 34.833 | 27.532 | 49.665 | 1.00 20.22 | |
| | 1132 | 0 | ILE A | 111 | 34.357 | 28.626 | 49.981 | 1.00 19.94 | AAAA |
| ATOM | | U | | | | | | | |
| ATOM | 1133 | N | ASN A | 145 | 34.787 | 26.451 | 50.440 | 1.00 20.57 | AAAA |
| | | | | | | 26.448 | 51.770 | 1.00 20.39 | AAAA |
| ATOM | 1134 | CA | ASN A | 143 | 34.165 | | | | |
| N TOOM | 1135 | CB | ASN A | 145 | 33.450 | 25.114 | 51.990 | 1.00 19.39 | AAAA |
| MOTA | | | | | | | | | |
| MOTA | 1136 | CG | ASN A | 145 | 32.505 | 25.143 | 53.171 | 1.00 19.31 | AAAA |
| | 1177 | 001 | ASN A | 145 | 32.862 | 25.583 | 54.263 | 1.00 21.26 | AAAA |
| MOTA | 1137 | | | | | | | | |
| ATOM | 1138 | ND2 | ASN A | 145 | 31.290 | 24.667 | 52.960 | 1.00 17.08 | - AAAA |
| | | | | | 35.236 | 26.621 | 52.856 | 1.00 20.17 | · AAAA |
| ATOM | 1139 | С | ASN A | 143 | | | | | |
| ATOM | 1140 | 0 | ASN A | 145 | 35.690 | 25.622 | 53.421 | 1.00 19.75 | AAAA |
| | | | | | | | | 1.00 20.06 | AAAA |
| ATOM | 1141 | N | ASN A | 140 | 35.644 | 27.862 | 53.148 | | |
| | 1142 | CA | ASN A | 146 | 36.671 | 28.075 | 54.166 | 1.00 20.98 | AAAA |
| ATOM | | | | | | | | | AAAA |
| ATOM | 1143 | CB | ASN A | 146 | 37.019 | 29.573 | 54.333 | 1.00 21.78 | |
| | 1144 | CG | ASN A | 115 | 35.876 | 30.411 | 54.882 | 1.00 22.78 | AAAA |
| MOTA | | | | | | | | | |
| ATOM | 1145 | OD1 | ASN A | 146 | 35.651 | 30.465 | 56.091 | 1.00 22.83 | AAAA |
| | | MINO | A CAT A | 116 | 35.144 | 31.078 | 53.983 | 1.00 23.70 | AAAA |
| ATOM | 1146 | NDZ | ASN A | 140 | | | | | |
| ATOM - | 1147 | С | ASN A | 146 | 36.307 | 27.413 | 55.496 | 1.00 21.18 | AAAA |
| | | | | | | 26.823 | 56.139 | 1.00 21.48 | AAAA |
| ATOM | 1148 | 0 | ASN A | 140 | 37.169 | | | | |
| ATOM | 1149 | N | PRO A | 147 | 35.031 | 27.476 | 55.922 | 1.00 20.88 | AAAA |
| | | | | | | | 55.358 | 1.00 21.85 | AAAA |
| ATOM | 1150 | CD | PRO A | 147 | 33.835 | 28.120 | 22.220 | | |
| | 1151 | CA | PRO A | 147 | 34.674 | 26.831 | 57.183 | 1.00 21.42 | AAAA |
| MOTA | | | | | | | | | AAAA |
| MOTA | 1152 | CB | PRO A | 147 | 33.176 | 27.073 | 57.261 | 1.00 21.00 | |
| | 1153 | CG | PRO A | 147 | 33.052 | 28.408 | 56.605 | 1.00 20.47 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 1154 | С | PRO. A | 147 | 35.015 | 25.334 | 57.174 | 1.00 22.79 | AAAA |
| | | | PRO A | | 35.650 | 24.833 | 58.099 | 1.00 25.69 | AAAA |
| ATOM | 1155 | 0 | | | | | | | |
| ATOM | 1156 | N | ALA A | 148 | 34.603 | 24:616 | 56.136 | 1.00 22.34 | AAAA |
| | | | | | 34.889 | 23.193 | 56.070 | 1.00 22.23 | AAAA |
| MOTA | 1157 | CA | ALA A | 740 | | | • | | |
| ATOM | 1158 | CB | ALA A | 148 | 34.260 | 22.561 | 54.825 | 1.00 22.87 | AAAA |
| | | | | | | | 56.054 | 1.00 22.33 | AAAA |
| ATOM | 1159 | С | ALA A | 148 | 36.378 | 22.998 | | | |
| | 1160 | 0 | ALA A | 148 | 36.912 | 22.249 | 56.861 | 1.00 23.42 | AAAA |
| ATOM | | | | | | | 55.122 | 1.00 22.50 | AAAA |
| MOTA | 1161 | N | VAL A | 149 | 37.050 | 23.661 | | | |
| | 1162 | CA | VAL A | 149 | 38.505 | 23.569 | 55.018 | 1.00 21.29 | AAAA |
| MOTA | | | | | | | 54.002 | 1.00 20.46 | AAAA |
| ATOM | 1163 | CB | VAL A | 149 | 39.066 | 24.581 | 54.002 | | |
| | 1164 | CCI | VAL A | 149 | 40.578 | 24.607 | 54.085 | 1.00 19.36 | AAAA |
| ATOM | | | | | | | | 1.00 20.03 | AAAA |
| ATOM | 1165 | CG2 | VAL A | 149 | 38.608 | 24.229 | 52.593 | | |
| | • | С | VAL A | 149 | 39.164 | 23.848 | 56.367 | 1.00 21.48 | AAAA |
| ATOM | 1166 | C | | | | | | | |
| ATOM | 1167 | 0 | VAL A | 149 | 40.147 | 23.197 | 56.735 | 1.00 22.11 | AAAA |
| | | | GL" A | | 38.628 | 24.826 | 57.088 | 1.00 21.19 | AAAA |
| ATOM | 1168 | N | | | | | | | |
| MOTA | 1169 | CA | GL A | 150 | 39.171 | 25.176 | 58.386 | 1.00 21.70 | |
| | | | | | 38.973 | 24.043 | 59.368 | 1.00 22.31 | AAAA |
| ATOM | 1170 | С. | GL'. A | | | | | | |
| MOTA | 1171 | 0 | GLY A | 150 | 39.913 | 23.597 | 60.026 | 1.00 22.51 | AAAA |
| | | | | | | 23.566 | 59.453 | 1.00 22.86 | AAAA |
| ATOM | 1172 | N | ILE A | | 37.736 | | | | |
| ATOM | 1173 | CA | ILE A | 151 | 37.388 | 22.474 | 60.346 | 1.00 22.26 | AAAA |
| | | | * | 101 | | | | 1.00 21.51 | AAAA |
| MOTA | 1174 | CB | ILE A | . 151 | 35.894 | 22.124 | | | |
| | 1175 | CG2 | ILE A | 151 | 35.542 | 20.899 | 61.019 | 1.00 21.36 | AAAA |
| MOTA | | COL | | | | | | 1.00 20.39 | AAAA |
| MOTA | 1176 | CG1 | ILE A | 151 | 35.051 | 23.329 | 60.627 | | |
| | | | ILE A | | 33.576 | 23.199 | 60.361 | 1.00 16.88 | AAAA |
| MOTA | 1177 | | | | | | | | |
| ATOM | 1178 | С | ILE A | 151 | 38.265 | 21.243 | 60.096 | 1.00 23.29 | AAAA |
| - | | | | | 38.786 | 20.660 | 61.038 | 1.00 23.88 | AAAA |
| ATOM | 1179 | 0 | ILE A | | | | | | |
| | 1180 | N | GLU A | 152 | 38.435 | 20.853 | 58.836 | 1.00 24.13 | AAAA |
| MOTA | | | | 150 | | | 58.517 | 1.00 25.01 | AAAA |
| MOTA | 1181 | CA | GLU A | 152 | 39.267 | 19.697 | | | |
| | | CB | GLU A | 152 | 39.242 | 19.404 | 57.010 | 1.00 25.07 | AAAA |
| atom | 1182 | | טדים ע | | | | | | AAAA |
| ATOM | 1183 | CG | GLU A | 152 | 37.910 | 18.886 | 56.526 | 1.00 24.56 | |
| | | | GLU A | | 37.500 | 17.570 | 57.198 | 1.00 25.00 | AAAA |
| ATOM | 1184 | CD | OLU A | | - | | | | |
| ATOM | 1185 | OE1 | GLU A | 152 | 36.345 | 17.158 | 57.011 | 1.00 26.40 | AAAA |
| | | 022 | GLU A | 150 | 38.315 | 16.935 | 57.897 | 1.00 25.00 | AAAA |
| ATOM | 1186 | UEZ | பூப A | | | | | | |
| ATOM | 1187 | C | GLU A | 152 | 40.694 | 19.957 | 58.965 | 1.00 26.06 | AAAA |
| | | | GLU A | 157 | 41.425 | 19.035 | 59.331 | 1.00 26.40 | . AAAA |
| ATOM | 1188 | 0 | GLU A | 104 | 41.423 | 19.000 | | | |
| | | | | | | | | | • |
| | | | | | | | | | |

| MOTA | 1189 | N | TYR A | 153 | 41.085 | 21.225 | 58.925 | 1.00 27.30 | AAAA |
|--------|------|-----|---------|-------------|--------|--------|--------|------------|--------------|
| MOTA | 1190 | CA | TYR A | 153 | 42.422 | | | 1.00 27.63 | AAAA |
| ATOM | 1191 | CE | TYR A | 153 | 42.532 | 23.153 | 59.268 | 1.00 26.99 | |
| MOTA | 1192 | CG | TYR A | 153 | 43.856 | 23.719 | 59.710 | 1.00 27.03 | AAAA |
| MOTA | 1193 | CD | 1 TYR A | 153 | 44.942 | 23.790 | 58.837 | 1.00 27.78 | |
| MOTA | 1194 | CE | 1 TYR A | 153 | 46.165 | 24.356 | 59.250 | 1.00 28.40 | |
| MOTA | 1195 | | 2 TYR A | 153 | 44.017 | 24.215 | 61.007 | 1.00 27.52 | |
| MOTA | 1196 | CE | | | 45.216 | 24.774 | 61.425 | 1.00 27.66 | |
| ATOM | 1197 | CZ | TYR A | 153 | 46.284 | 24.845 | 60.547 | 1.00 28.15 | |
| ATOM | 1198 | | | | 47.457 | 25.407 | 60.974 | 1.00 28.83 | AAAA |
| MOTA | 1199 | | TYR A | | 42.618 | 21.172 | 60.769 | 1.00 27.82 | |
| ATOM | 1200 | | TYR A | | 43.613 | 20.552 | 61.110 | 1.00 27.15 | AAAA |
| ATOM | 1201 | N | LEU A | | 41.636 | 21.487 | 61.604 | 1.00 29.25 | |
| ATOM | 1202 | | | | 41.665 | 21.138 | 63.014 | 1.00 29.35 | AAAA |
| MOTA | 1203 | CB | | | 40.507 | 21.829 | 63.715 | 1.00 30.25 | |
| MOTA | 1204 | CG | | | 40.685 | 23.346 | 63.792 | 1.00 31.10 | AAAA |
| ATOM | 1205 | | 1 LEU A | | 39.348 | 24.020 | 64.092 | 1.00 31.24 | |
| ATOM | 1206 | | 2 LEU A | | 41.747 | 23.669 | 64.852 | 1.00 29.84 | AAAA |
| MOTA | 1207 | C | LEU A | | 41.625 | 19.639 | 63.263 | 1.00 29.73 | |
| ATOM | 1208 | ō | LEU A | | 42.313 | 19.151 | 64.150 | 1.00 30.51 | AAAA |
| ATOM | 1209 | N | ARG A | | 40.832 | 18.903 | 62.489 | 1.00 28.95 | AAAA |
| ATOM | 1210 | CA | | | 40.771 | 17.459 | 62.671 | 1.00 28.94 | AAAA AAAA |
| ATOM | 1211 | CB | ARG A | | 39.742 | 16.820 | 61.723 | 1.00 28.64 | |
| ATOM | 1212 | CG | ARG A | | 38.312 | 17.312 | 61.952 | 1.00 27.82 | AAAA |
| ATOM | 1213 | CD | ARG A | | 37.319 | 16.751 | 60.955 | 1.00 27.19 | AAAA |
| ATOM | 1214 | NE | ARG A | | 36.804 | 15.444 | 61.338 | 1.00 27.19 | AAAA |
| MOTA | 1215 | CZ | ARG A | | 35.939 | 14.742 | 60.612 | 1.00 28.93 | . AAAA |
| ATOM | 1216 | | L ARG A | | 35.500 | 15.227 | 59.459 | 1.00 28.93 | AAAA AAAA |
| ATOM | 1217 | | ARG A | | 35.486 | 13.574 | 61.053 | 1.00 28.76 | AAAA |
| ATOM | 1218 | C | ARG A | | 42.158 | 16.853 | 62.438 | 1.00 30.20 | AAAA |
| ATOM | 1219 | Ö | ARG A | | 42.572 | 15.949 | 63.164 | 1.00 30.74 | AAAA |
| ATOM | 1220 | N | LYS A | | 42.890 | 17.362 | 61.447 | 1.00 30.32 | AAAA |
| ATOM | 1221 | CA | LYS A | | 44.224 | 16.838 | 61.173 | 1.00 30.07 | AAAA |
| ATOM | 1222 | CB | LYS A | | 44.771 | 17.373 | 59.847 | 1.00 30.26 | AAAA |
| ATOM | 1223 | CG | LYS A | | 46.168 | 16.869 | 59.525 | 1.00 30.16 | AAAA |
| ATOM | 1224 | CD | LYS A | | 46.686 | 17.368 | 58.181 | 1.00 31.19 | AAAA |
| ATOM | 1225 | CE | LYS A | | 45.884 | 16.813 | 56.986 | 1.00 31.70 | AAAA |
| ATOM | 1226 | NZ | LYS A | | 45.963 | 15.324 | | 1.00 31.20 | AAAA |
| MOTA | 1227 | С | LYS A 1 | 156 | 45.167 | 17.202 | 62.306 | 1.00 30.08 | AAAA |
| MOTA | 1228 | 0 | LYS A 1 | | 46.192 | 16.550 | 62.485 | 1.00 29.16 | AAAA |
| ATOM | 1229 | N | LYS A 1 | 157 | 44.816 | 18.252 | 63.053 | 1.00 30.08 | AAAA |
| MOTA | 1230 | CA | LYS A 1 | L57 | 45.608 | 18.691 | 64.196 | 1.00 31.03 | AAAA |
| MOTA | 1231 | CB | LYS A 1 | L 57 | 45.446 | 20.201 | 64.452 | 1.00 31.81 | AAAA |
| ATOM | 1232 | CG | LYS A 1 | 57 | 46.067 | 21.134 | 63.419 | 1.00 32.12 | AAAA |
| ATOM | 1233 | CD | LYS A 1 | 157 | 47.580 | 21.041 | 63.348 | 1.00 31.34 | AAAA |
| MOTA | 1234 | CE | LYS A 1 | .57 | 48.080 | 21.941 | 62.226 | 1.00 32.66 | AAAA. |
| MOTA | 1235 | NZ | LYS A 1 | .57 | 49.556 | 21.921 | 61.996 | 1.00 32.74 | \AAA |
| MOTA | 1236 | С | LYS A 1 | .57 | 45.196 | 17.923 | 65.458 | 1.00 31.73 | AAA' |
| MOTA | 1237 | O. | LYS A 1 | .57 | 45.652 | 18.230 | 66.558 | 1.00 31.93 | AAAA |
| ATOM | 1239 | N | GLY A 1 | .58 | 44.312 | 16.942 | 65.299 | 1.00 32.41 | AAAA |
| MOTA | 1239 | CA | GLY A 1 | .58 | 43.901 | 16.140 | 66.436 | 1.00 32.34 | AAAA |
| MOTA | 1240 | С | GLY A 1 | .58 | 42.604 | 16.429 | 67.172 | 1.00 32.65 | AAAA |
| ATOM | 1241 | 0 | GLY A 1 | 58 | 42.182 | 15.604 | 67.980 | 1.00 32.85 | AAAA |
| ATCM | 1242 | N | PHE A 1 | 59 | 41.960 | 17.565 | 66.932 | 1.00 33.16 | AAAA |
| MOTA | 1243 | CA | PHE A 1 | 59 | 40.712 | 17.842 | 67.650 | 1.00 34.16 | AAAA |
| MOTA | 1244 | CB | PHE A 1 | 59 | 40.220 | 19.281 | 67.403 | 1.00 34.81 | AAAA |
| ATOM | 1245 | CG | PHE A 1 | 59 | 41.134 | 20.343 | 67.965 | 1.00 34.01 | AAAA |
| MOTA | 1246 | CD1 | PHE A 1 | 59 | 42.327 | 20.669 | 67.329 | 1.00 34.18 | AAAA |
| ATOM | 1247 | | PHE A 1 | | 40.821 | 20.981 | 69.166 | 1.00 34.61 | AAAA |
| MOTA | 1248 | CE1 | PHE A 1 | 59 | 43.197 | 21.610 | 67.874 | 1.00 33.65 | AAAA |
| ATOM . | 1249 | CE2 | PHE A 1 | 59 | 41.689 | 21.924 | 69.718 | 1.00 34.52 | AAAA |
| MOTA | 1250 | CZ | PHE A 1 | 59 | 42.878 | 22.236 | 69.065 | 1.00 33.90 | AAAA |
| ATOM | 1251 | С | PHE A 1 | | 39.645 | 16.840 | 67.239 | 1.00 34.04 | AAAA |
| ATOM | 1252 | 0 | PHE A 1 | 59 | 39.568 | 16.456 | 66.068 | 1.00 34.98 | AAAA |
| ATOM | 1253 | N | LYS A 1 | | 38.839 | 16.403 | 68.202 | 1.00 33.36 | AAAA |
| ATOM | 1254 | CA | LYS A 1 | | 37.794 | 15.415 | 67.936 | 1.00 33.11 | AAAA |
| | | | | | | | - | | |

| | | | | | | • | | | | | |
|------|------|-----|-------|---|-------|---|--------|--------|--------|----------|----------|
| MOTA | 1255 | CB | LYS | А | 160 | | 38.060 | 14.140 | 68.763 | 1.00 33. | 97 AAAA |
| | | CG | | | 160 | | 39.410 | 13.491 | 68.457 | 1.00 35. | |
| MOTA | 1256 | | | | • | | | | | | |
| ATOM | 1257 | CD | | | 160 | | 39.833 | 12.364 | 69.429 | 1.00 36. | |
| ATOM | 1258 | CE | LYS | A | 160 | | 39.095 | 11.037 | 69.243 | 1.00 37. | 97 AAAA |
| MOTA | 1259 | NZ | LYS | Α | 160 | | 37.636 | 11.080 | 69.568 | 1.00 39. | 67 AAAA |
| | 1260 | C | | | 160 | | 36.385 | 15.941 | 68.210 | 1.00 31. | |
| MOTA | | | | | | | | | | | |
| ATOM | 1261 | 0 | LYS | A | 160 | | 35.405 | 15.290 | 67.887 | 1.00 31. | |
| ATOM | 1262 | N | ARG | Α | 161 | | 36.291 | 17.114 | 68.819 | 1.00 31. | 11 AAAA |
| ATOM | 1263 | CA | ARG | А | 161 | | 35.003 | 17.719 | 69.114 | 1.00 30. | 92 AAAA |
| | | CB | | | 161 | | 34.655 | 17.592 | 70.604 | 1.00 31. | |
| ATOM | 1264 | | | | | | | | | | |
| ATOM | 1265 | CG | ARG | A | 161 | | 34.451 | 16.157 | 71.102 | 1.00 32. | |
| ATOM | 1266 | CD | ARG | Α | 161 | | 33.994 | 16.126 | 72.570 | 1.00 33. | 26 AAAA |
| MOTA | 1267 | NE | ARG | A | 161 | | 34.929 | 16.797 | 73.476 | 1.00 34. | 01 AAAA |
| | 1268 | CZ | | | 161 | | 36.183 | 16.404 | 73.698 | 1.00 34. | |
| ATOM | | | | | | | | | | | |
| MOTA | 1269 | | ARG | | | | 36.675 | 15.334 | 73.081 | 1.00 34. | |
| ATOM | 1270 | NH2 | ARG | Α | 161 | | 36.954 | 17.084 | 74.537 | 1.00 34. | |
| ATOM | 1271 | С | ARG | Α | 161 | | 35.061 | 19.185 | 68.714 | 1.00 30. | 28 AAAA |
| | 1272 | 0 | | | 161 | | 35.365 | 20.059 | 69.529 | 1.00 29. | 86 AAAA |
| MOTA | | | | | | | | | 67.437 | 1.00 28. | |
| MOTA | 1273 | N | | | 162 | | 34.774 | 19.433 | | | |
| MOTA | 1274 | CA | ILE | A | 162 | | 34.788 | 20.774 | 66.862 | 1.00 26. | |
| ATOM | 1275 | CB | ILE | Α | 162 | | 35.443 | 20.762 | 65.464 | 1.00 26. | 87 AAAA |
| ATOM | 1276 | CG2 | ILE | Α | 162 | | 35.453 | 22.160 | 64.872 | 1.00 26. | 91 AAAA |
| | | | ILE | | | | 36.877 | 20.234 | 65.578 | 1.00 28. | |
| ATOM | 1277 | | | | | | | | | | |
| ATOM | 1278 | | ILE | | | | 37.614 | 20.090 | 64.240 | 1.00 28. | |
| MOTA | 1279 | С | ILE | Α | 162 | | 33.369 | 21.283 | 66.731 | 1.00 24. | |
| MOTA | 1280 | 0 | ILE | Α | 162 | | 32.485 | 20.572 | 66.267 | 1.00 24. | 40 AAAA |
| MOTA | 1281 | N | 1.511 | Δ | 163 | | 33.153 | 22.519 | 67.153 | 1.00 22. | 25 AAAA |
| | | | | | 163 | | 31.838 | 23.126 | 67.074 | 1.00 20. | |
| MOTA | 1282 | CA | | | | • | | | | | |
| ATOM | 1283 | CB | | | 163 | | 31.408 | 23.671 | 68.440 | 1.00 20. | |
| ATOM | 1284 | CG | LEU | Α | 163 | | 30.099 | 24.477 | 68.486 | 1.00 20. | 50 AAAA |
| ATOM | 1285 | CD1 | LEU | А | 163 | | 28.998 | 23.695 | 67.799 | 1.00 19. | 07 AAAA |
| | | | LEU | | | | 29.738 | 24.802 | 69.950 | 1.00 19. | 76 AAAA |
| ATOM | 1286 | | | | | | | | | 1.00 18. | |
| MOTA | 1287 | С | | | 163 | | 31.801 | 24.241 | 66.055 | | |
| ATOM | 1288 | 0 | LEU | A | 163 | | 32.756 | 24.986 | 65.894 | 1.00 18. | |
| MOTA | 1289 | N | TYR | Α | 164 | | 30.677 | 24.344 | 65.368 | 1.00 17. | 85 AAAA |
| ATOM | 1290 | CA | πVR | А | 164 | | 30.496 | 25.372 | 64.373 | 1.00 17. | 16 AAAA |
| | | CB | | | 164 | | 30.644 | 24.768 | 62.983 | 1.00 17. | 45 AAAA |
| ATOM | 1291 | | | | | | | | 61.900 | 1.00 17. | |
| ATOM | 1292 | CG | | | 164 | | 30.484 | 25.783 | | | |
| ATOM | 1293 | CD1 | TYR | A | 164 | | 31.444 | 26.772 | 61.701 | 1.00 16. | |
| ATOM | 1294 | CE1 | TYR | Α | 164 | | 31.280 | 27.734 | 60.721 | 1.00 17. | .35 AAAA |
| ATOM | 1295 | CD2 | TYR | A | 164 | | 29.350 | 25.781 | 61.092 | 1.00 17. | .95 AAAA |
| | 1296 | | TYR | | | | 29.173 | 26.746 | 60.103 | 1.00 18. | AAAA EO |
| ATOM | | | | | | | | | 59.919 | 1.00 17. | |
| MOTA | 1297 | CZ | | | 164 | | 30.138 | 27.717 | | | |
| MOTA | 1298 | OH | TYR | Α | 164 | | 29.955 | 28.647 | 58.926 | 1.00 16. | |
| ATOM | 1299 | С | TYR | A | 164 | | 29.123 | 26.016 | 64.514 | 1.00 15. | .85 AAAA |
| ATOM | 1300 | 0 | TYR | А | 164 | | 28.101 | 25.351 | 64.416 | 1.00 16. | 44 AAAA |
| | | Ň | | | 165 | | 29.115 | 27.319 | 64.743 | 1.00 15. | 54 AAAA |
| MOTA | 1301 | | | | | | | | | 1.00 15. | |
| ATOM | 1302 | | | | 165 • | • | 27.878 | 28.088 | 64.897 | | |
| ATOM | 1303 | CB | ILE | Α | 165 | | 27.869 | 28.819 | 66.250 | 1.00 15. | |
| ATOM | 1304 | CG2 | ILE | Α | 165 | | 26.621 | 29.685 | 66.374 | 1.00 13. | 94 AAAA |
| | 1305 | | ILE | _ | | | 28.000 | 27.797 | 67.386 | 1.00 13. | .94 AAAA |
| ATOM | | | | | | | 28.356 | 28.421 | 68.747 | 1.00 13. | |
| MOTA | 1306 | | ILE | | | | | | | | |
| ATOM | 1307 | С | | | 165 | | 27.808 | 29.124 | 63.754 | 1.00 16. | |
| ATOM | 1308 | 0 | ILE | Α | 165 | | 28.711 | 29.941 | 63.576 | 1.00 16. | .56 AAAA |
| ATOM | 1309 | N | ASP | А | 166 | | 26.721 | 29.087 | 63.001 | 1.00 16. | .18 AAAA |
| | | CA | ASP | | | | 26.524 | 29.962 | 61.865 | 1.00 16. | |
| ATOM | 1310 | | | | | | | | 60.651 | 1.00 18. | |
| MOTA | 1311 | CB | ASP | | | | 26.240 | 29.066 | | | |
| MOTA | 1312 | CG | ASP | A | 166 | | 26.238 | 29.809 | 59.329 | 1.00 19. | |
| ATOM | 1313 | OD1 | ASP | A | 166 | | 25.353 | 30.659 | 59.114 | 1.00 18. | |
| | 1314 | | ASP | | | | 27.131 | 29.521 | 58.495 | 1.00 19. | .19 AAAA |
| MOTA | | | | | | | | 30.904 | 62.169 | 1.00 17. | |
| MOTA | 1315 | C | ASP | | | | 25.342 | | | | |
| ATOM | 1316 | 0 | ASP | | | | 24.206 | 30.459 | 62.321 | 1.00 17: | |
| ATOM | 1317 | N . | LEU | A | 167 | | 25.605 | 32.202 | 62.274 | 1.00 16. | |
| ATOM | 1318 | CA | LEU | | | | 24.526 | 33.135 | 62.562 | 1.00 16. | AAAA e8 |
| | | CB | LEU | | | | 24.923 | 34.116 | 63.663 | 1.00 17. | .27 AAAA |
| MOTA | 1319 | | | | | | | | 64.954 | 1.00 18. | |
| ATOM | 1320 | CG | LEU | A | 10/ | | 25.499 | 33.529 | | 1.00 10. | , man |
| · · | | | | _ | | | | | | | |

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Figure 19-21

| MOTA | 1321 CD1 LE | U A 167 | 25.760 | 34.671 | 65.933 | 1.00 18.72 | AAAA |
|---------|--|---------|--------|--------|--------------------|-------------|------|
| MOTA | 1322 CD2 LE | U A 167 | 24.566 | | | 1.00 17.06 | |
| ATOM | | U A 167 | 24.146 | | | | AAAA |
| ATOM | | U A 167 | | | | 1.00 17.18 | AAAA |
| | | | 23.390 | | | 1.00 17.21 | AAAA |
| ATOM | | P A 168 | 24.683 | | 60.178 | 1.00 17.83 | AAAA |
| MOTA | | P A 168 | 24.382 | 34.067 | 58.904 | 1.00 17.84 | AAAA |
| MOTA | 132.7 CB ASI | P A 168 | 25.178 | 33.397 | | 1.00 20.42 | |
| MOTA | | P A 168 | 25.140 | | | 1 00 20.42 | AAAA |
| ATOM | | A. 168 | | | | 1.00 21.41 | AAAA |
| | | | 22.915 | | | 1.00 18.35 | AAAA |
| MOTA | | P A 168 | 22.419 | 32.722 | 59.032 | 1.00 19.62 | AAAA |
| MOTA | 1331 OD1 ASE | | 26.066 | 34.972 | 56.330 | 1.00 22.42 | AAAA |
| ATOM | 1332 OD2 ASE | A 168 | 24.186 | 33.971 | 55.746 | 1.00 21.79 | |
| · ATOM. | | A 169 | 22.239 | | 58.010 | | AAAA |
| ATOM | | A 169 | 20.824 | | | 1.00 17.98 | AAAA |
| ATOM | | A 169 | | | 57.708 | 1.00 17.36 | AAAA |
| | | | 20.348 | | 57.007 | 1.00 17.00 | AAAA |
| ATOM | | A 169 | 20.439 | 33.377 | 56.88 7 | 1.00 18.64 | AAAA |
| ATOM | 1337 O ALA | A 169 | 19,255 | 33.043 | 56.819 | 1.00 19.46 | AAAA |
| MOTA | 1338 N HIS | A 170 | 21.412 | 32.712 | 56.262 | 1.00 18.71 | AAAA |
| MOTA | | A 170 | 21.107 | 31.518 | 55.464 | | |
| ATOM | and the second s | A 170 | | | | 1.00 18.43 | AAAA |
| | | | 21.802 | 30.265 | 55.986 | 1.00 18.02 | AAAA |
| MOTA | | A 170 | 22.910 | 30.332 | 56.514 | 1.00 17.20 | AAAA |
| ATOM | | A 170 | 21.539 | 31.678 | 54.004 | 1.00 18.79 | AAAA |
| ATOM | 1343 CG HIS | A 170 | 21.137 | 32.968 | 53.386 | 1.00 17.65 | AAAA |
| ATOM | 1344 ND1 HIS | A 170 | 21.644 | 34.162 | 53.828 | 1.00 18.08 | |
| ATOM | 1345 CE1 HIS | | 21.112 | 35.081 | 53.054 | | AAAA |
| ATOM | 1346 CD2 HIS | | | | | 1.00 18.95 | AAAA |
| ATOM | 1347 NE2 HIS | | 20.301 | 33.194 | 52.348 | 1.00 18.81 | AAAA |
| | | | 20.291 | 34.544 | 52.140 | 1.00 19.66 | AAAA |
| MOTA | | A 171 | 21.142 | 29.124 | 55.793 | 1.00 17.53 | AAAA |
| MOTA | | A 171 | 21.662 | 27.822 | 56.193 | 1.00 16.38 | AAAA |
| ATOM | 1350 CB HIS | A 171 | 20.644 | 26.740 | 55.830 | 1.00 16.32 | AAAA |
| MOTA | 1351 CG HIS | ·A 171 | 21.157 | 25.337 | 55.958 | 1.00 15.91 | |
| ATOM | 1352 CD2 HIS | | 21.241 | 24.336 | 55.051 | | AAAA |
| ATOM | 1353 ND1 HIS | | | | | 1.00 14.14 | AAAA |
| | 1354 CE1 HIS | | 21.602 | 24.807 | 57.151 | 1.00 16.79 | AAAA |
| MOTA | | | 21.937 | 23.543 | 56.973 | 1.00 14.91 | AAAA |
| MOTA | 1355 NE2 HIS | | 21.725 | 23.234 | 55.709 | 1.00 15.45 | AAAA |
| ATOM | | A 171 | 22.982 | 27.522 | 55.509 | 1.00 16.94 | AAAA |
| MOTA | 1357 O HIS | A 171 | 23.146 | 27.725 | 54.318 | 1.00 18.71 | AAAA |
| ATOM | 1358 N CYS | A 172 | 23.926 | 27.019 | 56.279 | 1.00 16.99 | AAAA |
| ATOM | | A 172 | 25.237 | 26.670 | 55.778 | 1.00 16.23 | |
| ATOM | | A 172 | 26.219 | | | | AAAA |
| MOTA | | | | 26.721 | 56.947 | 1.00 17.89 | AAAA |
| | | A 172 | 25.638 | 25.773 | 58.397 | 1.00 17.89 | AAAA |
| MOTA | | A 172 | 25.205 | 25.271 | 55.210 | 1.00 16.57 | AAAA |
| ATOM | | A 172 | 25.947 | 24.413 | 55.670 | 1.00 17.66 | AAAA |
| MOTA | 1364 N ASP | A 173 | 24.364 | 25.026 | 54.214 | 1.00 18.25 | AAAA |
| ATOM | 1365 CA ASP | A 173 | 24.253 | 23.680 | 53.620 | 1.00 19.91 | AAAA |
| MOTA | | A 173 | 23.342 | 23.699 | 52.397 | 1.00 20.86 | |
| ATOM | | A 173 | 23.780 | | | | AAAA |
| | 1368 OD1 ASP | | | 24.719 | 51.358 | 1.00 21.90 | AAAA |
| ATOM | | - | 23.257 | 24.640 | 50.217 | 1.00 21.35 | AAAA |
| | 1369 OD2 ASP | | 24.624 | 25.597 | 51.687 | 1.00 21.35 | AAAA |
| ATOM | | A 173 | 25.573 | 23.021 | 53.227 | 1.00 21.02 | AAAA |
| ATOM | 1371 O ASP 2 | A 173 | 25.673 | 21.785 | 53.199 | 1.00 22.79 | |
| ATOM | | A 174 | 26.579 | 23.832 | 52.912 | 1.00 20.03 | AAAA |
| ATOM | | A 174 | 27.870 | | | | AAAA |
| | | | | 23.277 | 52.553 | 1.00 19.72 | AAAA |
| ATOM | | A 174 | 28.537 | 22.680 | 53.771 | 1.00 20.27 | AAAA |
| ATOM | 1375 O GLY A | | 29.110 | 21.599 | 53.711 | 1.00 19.77 | AAAA |
| ATOM | · | 3 175 · | 28.448 | 23.387 | 54.893 | 1.00 21.38 | AAAA |
| ATOM | 1377 CA VAL A | 175 | 29.056 | 22.934 | 56.135 | 1.00 22.26 | AAAA |
| ATOM | 1378 CB VAL A | | 29.032 | 24.040 | 57.203 | 1.00 23.15 | |
| ATOM | 1379 CG1 VAL A | | 29.853 | 23.617 | | | AAAA |
| | | | | | 58.418 | 1.00 22.84 | AAAA |
| ATOM | 1380 CG2 VAL A | | 29.562 | | 56.612 | 1.00 23.43 | AAAA |
| MOTA | 1381 C VAL A | | 28.302 | 21.724 | 56.654 | 1.00 23.51 | AAAA |
| ATOM | 1382 O VAL A | 175 | 28.893 | 20.803 | 57.210 | 1.00 23.74 | AAAA |
| ATOM | 1383 N GLN A | 176 | 26.993 | 21.721 | 56.452 | 1.00 24.80 | AAAA |
| ATOM | 1384 CA GLN A | | 26.171 | 20.601 | 56.893 | 1.00 25.41 | |
| | | | | | | | AAAA |
| ATOM | | | 24.689 | | | 1.00 24.77. | AAAA |
| ATOM | 1386 CG GLN A | . T/0 | 23.799 | 19.735 | 57.036 | 1.00 26.23 | AAAA |

| MOTA | 1387 | CD | GLN A | A 1 | 76 | 22.334 | 20.094 | 57.069 | 1.00 27.17 | AAAA |
|-----------------------|------|------|--------|------------|-------------|--------|---------|----------------|-------------|--------|
| ATOM | 1388 | OE1 | GLN A | A 1 | .76 | 21.902 | 20.879 | 57.911 | 1.00 28.24 | AAAA |
| ATOM | 1389 | | GLN : | | | 21.556 | 19.522 | 56.151 | 1.00 26.54 | AAAA |
| | 1390 | C | GLN A | | | 26.512 | 19.293 | 56.180 | 1.00 25.67 | AAAA |
| ATOM | | | | | | 26.789 | 18.285 | 56.820 | 1.00 26.98 | AAAA |
| MOTA | 1391 | 0 | GLN : | | | | | 54.853 | 1.00 26.34 | AAAA |
| MOTA | 1392 | N | GLU | | | 26.490 | 19.309 | | | |
| MOFA | 1393 | CA | GLU . | A 1 | .77 | 26.786 | 18.117 | 54.073 | 1.00 26.18 | AAAA |
| MOTA | 1394 | CB | GLU . | A 1 | .7 7 | 26.746 | 18.468 | 52.580 | 1.00 27.13 | AAAA |
| ATOM | 1395 | CG | GLU . | | | 26.769 | 17.269 | 51.628 | 1.00 29.77 | AAAA |
| _ | | | _GLU . | | | 26.623 | 17.660 | 50.147 | 1.00 31.29 | AAAA |
| MOTA | 1396 | | | | | 27.655 | 17.935 | 49.500 | 1.00 31.35 | AAAA |
| ATOM | 1397 | | GLU . | | | | | | 1.00 32.05 | AAAA |
| MOTA | 1398 | OE2 | GLU . | | | 25.471 | 17.703 | 49.636 | | |
| MOTA | 1399 | C | GLU . | A l | .77 | 28.160 | 17.556 | 54.460 | 1.00 26.38 | AAAA |
| ATOM | 1400 | 0 | GLU . | A 1 | .77 | 28.338 | 16.349 | 54.595 | 1.00 25.41 | AAAA |
| ATOM | 1401 | N | ALA . | | | 29.115 | 18.458 | 54.659 | 1.00 -27.58 | AAAA |
| | 1402 | CA | ALA | | | 30.495 | 18.119 | 55.004 | 1.00 27.66 | - AAAA |
| MOTA | | | - | | | 31.345 | 19.385 | 54.994 | 1.00 26.20 | AAAA |
| MOTA | 1403 | CB | ALA . | | | | | 56.318 | 1.00 28.33 | AAAA |
| MOTA | 1404 | С | ALA | | | 30.713 | 17.370 | | | |
| MOTA | 1405 | 0 | ALA | A 1 | | 31.685 | 16.626 | 56.439 | 1.00 29.44 | AAAA |
| ATOM | 1406 | N | PHE | A 3 | 179 | 29.849 | 17.564 | 57.308 | 1.00 28.25 | AAAA |
| ATOM | 1407 | CA | PHE | A 1 | 179 | 30.036 | 16.852 | 58.561 | 1.00 29.20 | AAAA |
| | 1408 | CB | PHE | | | 30.570 | 17.794 | 59.624 | 1.00 29.35 | AAAA |
| MOTA | | | PHE | | | 31.751 | 18.572 | 59.171 | 1.00 30.26 | AAAA |
| MOTA | 1409 | CG | | | | | 19.777 | 58.497 | 1.00 31.01 | AAAA |
| MOTA | 1410 | | .PHE | | | 31.582 | | | 1.00 30.37 | AAAA |
| MOTA | 1411 | | PHE | | | 33.033 | 18.069 | 59.339 | | |
| ATOM | 1412 | CE1 | PHE | A] | 179 | 32.670 | 20.470 | 57.993 | 1.00 31.20 | AAAA |
| ATOM | 1413 | CE2 | PHE | A 1 | 179 | 34.133 | 18.749 | 58.840 | 1.00 31.74 | AAAA |
| ATOM | 1414 | CZ | PHE | | | 33.950 | 19.960 | 58.161 | 1.00 31.81 | AAAA |
| | 1415 | č | PHE | | | 28.760 | 16.180 | 59.040 | 1.00 30.33 | AAAA |
| MOTA | | | | | | 28.624 | 15.810 | 60.215 | 1.00 31.82 | AAAA |
| ATOM | 1416 | 0 | PHE | | | | | 58.105 | 1.00 29.18 | AAAA |
| MOTA | 1417 | N | TYR | | | 27.842 | 15.994 | | 1.00 28.99 | AAAA |
| ATOM | 1418 | CA | TYR | | | 26.564 | 15.379 | 58.389 | | |
| ATOM | 1419 | CB | TYR | A 1 | 180 | 25.725 | 15.343 | 57.123 | 1.00 28.30 | AAAA |
| ATOM | 1420 | CG | TYR | A : | 180 . | 24.244 | 15.422 | 57.384 | 1.00 28.27 | AAAA |
| MOTA | 1421 | | TYR | | | 23.392 | 14.386 | 57.021 | 1.00 27.05 | AAAA |
| | 1422 | CEI | | | | 22.029 | 14.491 | 57.197 | 1.00 28.51 | AAAA |
| ATOM | | | | | | 23.686 | 16.573 | 57.942 | 1.00 29.34 | AAAA |
| MOTA | 1423 | | TYR | | | 22.316 | 16.691 | 58.125 | 1.00 29.27 | AAAA |
| MOTA | 1424 | | TYR | | | | | | 1.00 29.33 | AAAA |
| ATOM | 1425 | CZ | TYR | Α. | 180 | 21.495 | 15.645 | 57.746 | | |
| MOTA | 1426 | OH | TYR | A : | 180 | 20.141 | 15.775 | 57.893 | 1.00 30.83 | AAAA |
| ATOM | 1427 | С | TYR | A : | 180 | 26.673 | 13.970 | 58.940 | 1.00 28.79 | AAAA |
| | 1428 | ō | TYR | | | 25.877 | 13.577 | 59.785 | 1.00 28.71 | AAAA |
| ATOM | | | ASP | | | 27.662 | 13.214 | 58.472 | 1.00 29.03 | AAAA |
| MOTA | 1429 | N | | | | 27.813 | 11.828 | 58.914 | 1.00 28.49 | AAAA |
| MOTA | 1430 | CA | ASP | | | | | 57.715 | 1.00 27.59 | AAAA |
| MOTA | 1431 | CB | ASP | | | 28.140 | 10.930 | | | AAAA |
| MOTA | 1432 | CG | ASP | A : | 181 | 29.548 | 11 122 | 57.229 | 1.00 28.82 | |
| ATOM | 1433 | OD1 | ASP | A : | 181 | 29:981 | 12 292 | 57.183 | 1.00 29.25 | AAAA |
| ATOM | 1434 | OD2 | ASP | A : | 181 | 30.216 | ,10 119 | 56.8 87 | 1.00 28.68 | AAAA |
| | | c | ASP | | | 28.863 | 11.631 | 60.009 | 1.00 27.67 | AAAA |
| ATOM | 1435 | | ASP | | | 29.271 | 10.504 | 60.293 | 1.00 27.57 | AAAA |
| ATOM | 1436 | 0 | | | | 20.272 | 12.713 | | 1.00 26.27 | AAAA |
| ATOM | 1437 | N | THR | | | | 12.713 | 61 699 | 1.00 26.22 | AAAA |
| ATCM | 1438 | CA | THR | A : | 182 | 30.284 | 12.544 | 61.689 | | |
| ATOM | 1439 | CB | THR | Α. | 182 | 31.670 | 13.118 | 61.317 | 1.00 25.92 | AAAA |
| | 1440 | | THR | | | 32.564 | 12.935 | 62.416 | 1.00 25.06 | AAAA |
| ATOM | | | THR | | | 31.577 | 14.594 | 60.974 | 1.00 25.25 | AAAA |
| ATOM | 1441 | | | | | 29.792 | 13.223 | 62.934 | 1.00 25.87 | AAAA |
| ATOM | 1442 | C | THR | | | | 14.102 | 62.863 | 1.00 26.35 | AAAA |
| ATOM | 1443 | 0 | THR | | | 28.942 | | | 1.00 25.86 | AAAA |
| ATOM | 1444 | 17 | ASP | | | 30.327 | 12.804 | 64.071 | | |
| ATOM | 1445 | CA | ASP | A | 183 | 29.953 | 13.370 | 65.355 | 1.00 26.12 | AAAA |
| | 1446 | CB | ASP | | | 29.468 | 12.260 | 66.274 | | AAAA |
| ATOM | | CG | ASP | | | 30.515 | 11.194 | 66.488 | 1.00 28.80 | AAAA |
| ATOM | 1447 | CG - | ASP | | | 31.063 | 10.691 | 65.480 | | AAAA |
| ATCM | 1448 | ODI | ASP | ~ | 103 | | 10.852 | 67.657 | | AAAA |
| ATOM | 1449 | OD2 | ASP | A | 192 | 30.781 | | | | AAAA |
| ATCM | 1450 | С | ASP | | | 31.126 | 14.120 | 65.995 | | |
| ATOM | 1451 | 0 | ASP | Α | 183 | 31.034 | 14.566 | 67.146 | | AAAA |
| and the second second | 1452 | N | GLN | A | 184 | 32.229 | 14.254 | 65,254 | 1.00 26.05 | AAAA |
| atom | 1372 | | . 65 | 30 | | CHE | | . DE \ | | • |

| ATOM | 1453 | CA | GLN | A 184 | 33.381 | 14.983 | CE 366 | | |
|-------|------|-----|-------|-------|--------|---------|-----------------|------------|------|
| ATOM | 1454 | | | A 184 | | | | 1.00 25.85 | AAAA |
| ATOM | 1455 | | | A 184 | 34.674 | | | | AAAA |
| ATOM | 1456 | | | | 34.920 | | | 1.00 27.42 | AAAA |
| | | | | A 184 | 36.273 | | 64.822 | 1.00 28.40 | AAAA |
| MOTA | 1457 | OE. | l GLN | A 184 | 36.685 | 12.905 | 63.709 | 1.00 30.05 | AAAA |
| ATOM | 1458 | | GLN | | 36.970 | 11.816 | 65.651 | 1.00 29.24 | AAAA |
| Mota | 1459 | C | GLN | A 184 | 33.159 | 16.474 | 65.536 | 1.00 25.22 | |
| ATOM | 1460 | 0 | GLN . | A 184 | 33.734 | | | 1.00 24.57 | AAAA |
| ATOM | 1461 | N | VAL . | A 185 | 32.290 | | 64.584 | 1.00 25.17 | AAAA |
| MOTA | 1462 | CA | | A 185 | 31.975 | | 64.291 | 1.00 23.17 | AAAA |
| ATOM | 1463 | CB | | A 185 | 32.324 | | | 1.00 24.49 | AAAA |
| ATOM | 1464 | | VAL | A 185 | 32.045 | | 62.832 | 1.00 23.20 | AAAA |
| ATOM | 1465 | CG2 | VAL | A 105 | | | 62.599 | 1.00 19.72 | AAAA |
| ATOM | 1466 | | | A 185 | 33.777 | | 62.543 | 1.00 20.67 | AAAA |
| ATOM | 1467 | | | A 185 | 30.494 | | 64.501 | 1.00 24.81 | AAAA |
| ATOM | | | | | 29.664 | | 63.844 | 1.00 27.07 | AAAA |
| | 1468 | | | A 186 | 30.162 | 19.311 | 65.434 | 1.00 23.40 | AAAA |
| ATOM | 1469 | | | A 186 | 28.768 | 19.645 | 65.684 | 1.00 20.31 | AAAA |
| ATOM | 1470 | | | A 186 | 28.513 | 19.937 | 67.164 | 1.00 19.77 | AAAA |
| MOTA | 1471 | | | A 186 | 27.057 | 20.037 | 67.500 | 1.00 18.55 | AAAA |
| MOTA | 1472 | CD1 | PHE A | A 186 | 26.359 | 18.918 | 67.945 | 1.00 17.70 | AAAA |
| MOTA | 1473 | | PHE A | | 26.358 | 21.213 | 67.263 | 1.00 17.46 | AAAA |
| MOTA | 1474 | CE1 | PHE A | A 186 | 24.999 | 18.964 | 68.147 | 1.00 17.35 | |
| MOTA | 1475 | CE2 | PHE A | A 186 | 24.997 | 21.271 | 67.459 | 1.00 18.83 | AAAA |
| MOTA | 1476 | CZ | PHE A | | | -20.138 | 67.905 | | AAAA |
| MOTA | 1477 | С | | 186 | 28.464 | 20.911 | 64.895 | 1.00 18.67 | AAAA |
| ATOM | 1478 | 0 | PHE A | | 29.079 | 21.940 | 65.129 | 1.00 19.18 | AAAA |
| MOTA | 1479 | N | VAL A | | 27.520 | | | 1.00 18.82 | AAAA |
| ATOM | 1480 | CA | VAL A | | 27.137 | 20.834 | 63.964 | 1.00 18.34 | AAAA |
| ATOM | 1481 | CB | VAL A | | | 21.993 | 63.160 | 1.00 16.47 | AAAA |
| ATOM | 1482 | | VAL A | | 27.006 | 21.630 | 61.655 | 1.00 14.30 | AAAA |
| ATOM | 1483 | | VAL A | | 26.628 | 22.869 | 60.828 | 1.00 10.34 | AAAA |
| ATOM | 1484 | C | | | 28.314 | 21.031 | 61.160 | 1.00 12.07 | AAAA |
| | | | VAL A | | 25.806 | 22.511 | 63.665 | 1.00 17.43 | AAAA |
| MOTA | 1485 | 0 | VAL A | | 24.852 | 21.746 | 63.792 | 1.00 16.95 | AAAA |
| MOTA | 1486 | N | LEU A | | 25.763 | 23.809 | 63.960 | 1.00 18.66 | AAAA |
| MOTA | 1487 | CA | LEU A | | 24.555 | 24.507 | 64.460 | 1.00 20.51 | AAAA |
| ATOM | 1488 | CB | LEU A | | 24.752 | 24.995 | 65.914 | 1.00 21.24 | AAAA |
| ATOM | 1489 | CG | LEU A | | 23.702 | 26.019 | 66.395 | 1.00 20.80 | AAAA |
| MOTA | 1490 | | LEU A | | 22.365 | 25.323 | 66.493 | | AAAA |
| ATOM | 1491 | | LEU A | | 24.085 | 26.627 | 67.750 | 1.00 20.63 | AAAA |
| MOTA | 1492 | С | LEU A | | 24.297 | 25.735 | 63.591 | 1.00 20.41 | AAAA |
| ATOM | 1493 | 0 | LEU A | | 25.223 | 26.484 | 63.288 | 1.00 21.86 | AAAA |
| MOTA | 1494 | N | SER A | | 23.049 | 25.987 | 63.233 | 1.00 19.32 | AAAA |
| ATOM | 1495 | CA | SER A | 189 | 22.786 | 27.130 | 62.381 | 1.00 18.06 | AAAA |
| ATOM | 1496 | CB | SER A | 189 | 22.970 | 26.715 | 60.906 | 1.00 18.54 | |
| ATOM | 1497 | OG | SER A | 189 | 22.559 | 27.731 | 59.998 | 1.00 17.47 | AAAA |
| MOT A | 1498 | С | SER A | 189 | 21.418 | 27.751 | 62.554 | 1.00 17.90 | AAAA |
| MOLE | 1499 | 0 | SER A | 189 | 20.404 | 27.051 | 62.540 | 1.00 17.90 | AAAA |
| A_OM | 1500 | N | LEU A | | 21.386 | 29.067 | 62.722 | 1.00 19.54 | AAAA |
| ATOM | 1501 | | LEU A | | 20.117 | 29.772 | 62.797 | 1.00 16.97 | AAAA |
| ATOM | 1502 | CB | LEU A | | 20.097 | | | 1.00 18.49 | AAAA |
| ATOM | 1503 | | LEU A | | | 30.865 | 63.886 | 1.00 17.78 | AAAA |
| ATOM | 1504 | | LEU A | | 20.534 | 30.600 | | 1.00 17.10 | AAAA |
| MOTA | 1505 | | LEU A | | 19.643 | 31.406 | 66.266 | 1.00 15.50 | AAAA |
| | | | | | 20.455 | 29.147 | 65.686 | 1.00 15.15 | AAAA |
| ATOM | 1506 | | LEU A | | 20.111 | 30.408 | 61.416 . | 1.00 19.35 | AAAA |
| ATOM | 1507 | | LEU A | | 21.136 | 30.891 | 60.967 | 1.00 19.75 | AAAA |
| ATOM | 1508 | | HIS A | | 18.975 | 30.397 | 60.736 | 1.00 21.75 | AAAA |
| MOTA | 1509 | | HIS A | | 18.897 | 30.955 | 59.383 | 1.00 23.55 | AAAA |
| MOTA | 1510 | | HIS A | | 19.626 | 30.013 | 58.426 | 1.00 23.63 | AAAA |
| ATOM | 1511 | | HIS A | | 19.157 | 28.597 | 58.533 | 1.00 24.26 | AAAA |
| MOTA | 1512 | | HIS A | | 19.770 | 27.485 | 59.009 | 1.00 23.78 | AAAA |
| ATOM | 1513 | ND1 | HIS A | 191 | 17.869 | 28.217 | 58.217 | 1.00 24.73 | |
| MOTA | 1514 | | HIS A | | 17.709 | 26.935 | 58.491 | 1.00 23.90 | AAAA |
| ATOM | 1515 | | HIS A | | 18.849 | 26.467 | 58.973 | | AAAA |
| ATOM | 1516 | | HIS A | | 17.446 | 31.119 | 58.926 | 1.00 24.51 | AAAA |
| ATOM | 1517 | | HIS A | | 16.519 | | 59.596 | 1.00 24.10 | AAAA |
| MOTA | 1518 | | GLN A | | 17.249 | 30.658 | | 1.00 24.94 | AAAA |
| ATOM. | 1310 | (| JAN A | | 11.247 | 31.789 | 57.794 | 1.00 24.33 | AAAA |
| | | | | | | | | | |

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Figure 19-24

| ATOM | 1519 | CA | GLN A | 192 | 15.899 | 31.959 | 57.269 | 1.00 25.77 | 7777 |
|--------|--------|-----|-------|-------|--------|--------|------------|------------|--------|
| ATOM | 1520 | CB | | | | | _ | | AAAA |
| | | | GĻN A | | 15.881 | 32.896 | 56.060 | 1.00 26.51 | AAAA |
| ATOM | 1521 | CG | GLN A | | 16.467 | 34.271 | 56.325 | 1.00 26.99 | AAAA |
| ATOM | 1522 | CD | GLN A | | 16.581 | 35.076 | 55.062 | 1.00 27.98 | AAAA |
| ATOM | 1523 | | GLN A | | 15.583 | 35.496 | 54.493 | 1.00 30.48 | AAAA |
| MOTA | 1524 | NE2 | GLN A | 192 | 17.802 | 35.274 | 54.595 | 1.00 29.04 | AAAA |
| ATOM | 1525 | С | GLN A | 192 | 15.463 | 30.573 | 56.832 | 1.00 25.77 | AAAA |
| ATOM . | 1526 | 0 | GLN A | 192 | 16.211 | 29.865 | 56.169 | 1.00 26.73 | AAAA |
| ATOM | 1527 | N | SER A | | 14.259 | 30.184 | 57.214 | 1.00 25.48 | AAAA |
| ATOM | 1528 | CA | SER A | | 13.750 | | | | |
| | | | | | | 28.877 | 56.863 | 1.00 24.51 | AAAA |
| ATOM | 1529 | CB | SER A | | 12.288 | 28.788 | 57.286 | 1.00 23.77 | AAAA |
| ATOM | 1530 | OG | SER A | | 11.753 | 27.517 | 57.010 | 1.00 24.81 | AAAA |
| MOTA | 1531 | C | SER A | | 13.906 | 28.597 | 55.361 | 1.00 24.53 | AAAA |
| MOTA | 1532 | 0 | SER A | . 193 | 13.736 | 29.479 | 54.522 | 1.00 22.32 | AAAA |
| MOTA | 1533 | N | PRO A | 194 | 14.226 | 27.348 | 55.007 | 1.00 25.69 | AAAA |
| ATOM | 1534 | CD | PRO A | 194 | 14.411 | 26.167 | 55.862 | 1.00 25.02 | AAAA |
| ATOM | 1535 | CA | PRO A | 194 | 14.399 | 26.976 | 53.604 | 1.00 27.05 | AAAA |
| MOTA | 1536 | CB | PRO A | | 14.906 | 25.535 | 53.697 | 1.00 26.30 | AAAA |
| MOTA | 1537 | CG | PRO A | | 15.479 | 25.466 | 55.124 | 1.00 26.44 | AAAA |
| | 1538 | C | PRO A | | 13.076 | 27.057 | 52.849 | | |
| MOTA | | | | | | | | 1.00 27.79 | AAAA |
| MOTA | 1539 | 0 | PRO A | | 13.066 | 27.057 | 51.625 | 1.00 28.82 | AAAA |
| atom | 1540 | N | GLU A | | 11.966 | 27.133 | 53.582 | 1.00 28.29 | AAAA |
| MOTA | 1541 | CA | GLU A | | 10.656 | 27.187 | 52.950 | 1.00 29.08 | AAAA |
| MOTA | 1542 | CB | GLU A | | 9.534 | 27.030 | 54.001 | 1.00 31.08 | AAAA |
| ATOM | 1543 | CG | GLU A | 195 | 9.070 | 28.294 | 54.722 | 1.00 35.07 | AAAA |
| MOTA | 1544 . | CD | GLU A | 195 | 7.850 | 28.980 | 54.064 | 1.00 38.05 | AAAA |
| ATOM | 1545 | OE1 | GLU A | 195 | 7.389 | 30.017 | 54.601 | 1.00 38.80 | AAAA |
| MOTA | 1546 | OE2 | GLU A | 195 | 7.342 | 28.487 | 53.024 | 1.00 39.20 | AAAA |
| ATOM | 1547 | С | GLU A | 195 | 10.483 | 28.471 | 52.150 | 1.00 28.05 | AAAA |
| ATOM | 1548 | Ó | GLU A | | 9.722 | 28.512 | 51.189 | 1.00 28.57 | AAAA |
| ATOM | 1549 | N | TYR A | | 11.223 | 29.510 | 52.514 | 1.00 27.39 | AAAA |
| MOTA | 1550 | CA | TYR A | | 11.108 | 30.769 | 51.802 | 1.00 25.80 | AAAA |
| ATOM | 1551 | СВ | TYR A | | 10.275 | 31.743 | 52.645 | 1.00 24.97 | AAAA |
| ATOM | 1552 | CG | TYR A | | 10.971 | 32.281 | 53.868 | 1.00 23.41 | AAAA |
| | | | TYR A | | 11.911 | 33.306 | 53.765 | 1.00 23.41 | |
| ATOM | 1553 | | | | | | | | AAAA |
| ATOM | 1554 | | TYR A | | 12.559 | 33.805 | 54.892 | 1.00 23.44 | AAAA |
| ATOM | 1555 | | TYR A | | 10.697 | 31.768 | 55.126 | 1.00 23.24 | AAAA |
| MOTA | 1556 | | TYR A | | 11.336 | 32.256 | 56.254 | 1.00 23.93 | AAAA |
| ATOM | 1557 | CZ | TYR A | | 12.265 | 33.270 | 56.133 | 1.00 24.07 | AAAA |
| ATOM | 1558 | OH | TYR A | | 12.913 | 33.731 | 57.247 | 1.00 25.06 | AAAA |
| ATOM | 1559 | С | TYR A | 196 | 12.450 | 31.406 | 51.411 | 1.00 24.97 | AAAA |
| ATOM | 1560 | 0 | TYR A | 196 | 12.475 | 32.495 | 50.840 | 1.00 25.14 | AAAA |
| MOTA | 1561 | N | ALA A | 197 | 13.563 | 30.737 | 51.686 | 1.00 23.81 | AAAA |
| ATOM | 1562 | CA | ALA A | 197 | 14.855 | 31.330 | 51.337 | 1.00 23.32 | AAAA |
| ATOM | 1563 | CB | ALA A | 197 | 15.350 | 32.220 | 52.488 | 1.00 23.33 | AAAA |
| ATOM - | 1564 | С | ALA A | | 15.952 | 30.356 | 50.957 | 1.00 22.74 | AAAA |
| MOTA | 1565 | | ALA A | | 15.951 | | .51 . 37 ' | 1.00 22.47 | AAAA |
| ATOM - | 1566 | | PHE A | | 16,900 | 30.852 | 50.16 | 1.00 23.23 | AAAA |
| ATOM | 1567 | CA | PHE A | | 18.062 | 30.081 | 49.741 | 1.00 23.68 | AAAA |
| | | CB | PHE A | | 19.083 | 31.006 | 49.069 | 1.00 23.33 | AAAA |
| MOTA | 1568 | | | | | | | 1.00 22.98 | |
| ATOM | 1569 | CG | PHE A | | 20.250 | 30.280 | 48.464 | | AAAA |
| ATOM | 1570 | | PHE A | | 20.151 | 29.713 | 47.203 | 1.00 22.75 | AAAA |
| ATOM | 1571 | | PHE A | | 21.436 | 30.127 | 49.175 | 1.00 23.32 | AAAA |
| MOTA | 1572 | | PHE A | | 21.207 | 29.003 | 46.645 | 1.00 22.13 | AAAA |
| ATOM | 1573 | | PHE A | | 22.512 | 29.408 | 48.622 | 1.00 22.83 | AAAA |
| MOTA | 1574 | CZ | PHE A | 198 | 22.386 | 28.849 | 47.351 | | AAAA . |
| ATOM | 1575 | С | PHE A | | 18.689 | 29.490 | 51.008 | 1.00 23.69 | AAAA |
| ATOM | 1576 | 0 | PHE A | 198 | 18.802 | 30.171 | 52.012 | 1.00 22.85 | AAAA |
| MOTA | 1577 | N | PRO A | | 19.166 | 28.236 | 50.954 | 1.00 23.96 | AAAA |
| MOTA | 1578 | CD | PRO A | | 19.833 | 27.639 | 52.123 | 1.00 24.26 | AAAA |
| ATOM | 1579 | CA | PRO A | | 19.199 | 27.286 | 49.837 | 1.00 24.70 | AAAA |
| ATOM | 1580 | CB | PRO A | | 20.163 | 26.222 | 50.357 | 1.00 23.30 | AAAA |
| | | CG | PRO A | | 19.797 | 26.162 | 51.782 | 1.00 23.21 | AAAA |
| ATOM | 1581 | | PRO A | | | 26.679 | 49.326 | 1.00 25.22 | AAAA |
| ATOM | 1582 | C | | | 17.885 | | 48.215 | 1.00 25.22 | |
| ATOM | 1583 | 0 | PRO A | | 17.866 | 26.145 | | | AAAA |
| ATOM | 1584 | N | PHE A | 200 | 16.811 | 26.756 | 50.116 | 1.00 25.09 | AAAA |

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| ATOM | 1585 | CA | PHE | А | 200 | | 15.497 | 26.190 | 49.763 | 1.00 26.29 | AAAA |
|--------------|--------------|------|-----|---|-----|---|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1586 | CB | PHE | | | | 15.064 | 26.567 | 48.340 | 1.00 25.65 | AAAA |
| ATOM | 1587 | CG | PHE | | | | 14.863 | 28.035 | 48.122 | 1.00 24.65 | AAAA |
| ATOM | 1588 | | PHE | | | | 15.806 | 28.781 | 47.439 | 1.00 24.42 | AAAA |
| MOTA | 1589 | | PHE | | | | 13.735 | 28.671 | 48.608 | 1.00 23.79 | AAAA |
| ATOM. | 1590 | | PHE | | | | 15.631 | 30.125 | 47.246 | 1.00 24.41 | AAAA |
| MOTA | 1591 | | PHE | | | | 13.552 | 30.035 | 48.418 | 1.00 24.94 | AAAA |
| ATOM | 1592 | CZ | PHE | | | | 14.499 | 30.760 | 47.738 | 1.00 24.57 | 'AAAA |
| | 1593 | C | PHE | | | | 15.415 | 24.656 | 49.863 | 1.00 28.54 | AAAA |
| MOTA | 1594 | Ö | PHE | | | | 14.386 | 24.096 | 50.251 | 1.00 28.76 | AAAA |
| MOTA | | И | GLU | | | | 16.499 | 23.981 | 49.504 | 1.00 29.67 | AAAA |
| MOTA | 1595 | CA | GLU | | | | 16.539 | 22.528 | 49.524 | 1.00 23.07 | AAAA |
| MOTA | 1596 | CB | GLU | | | _ | 17.434 | 22.045 | 48.392 | 1.00 31.00 | AAAA |
| ATOM | 1597 1598 | CG | GLU | | | | 16.897 | 22.415 | 47.017 | 1.00 34.87 | AAAA |
| MOTA | 1598 | CD | GLU | | | | 17.898 | 22.147 | 45.912 | 1.00 35.14 | AAAA |
| MOTA | - | | GLU | | | | 18.299 | 20.982 | 45.735 | 1.00 35.14 | - AAAA |
| MOTA | 1600 | | | | | | | . 23.112 | 45.221 | 1.00 36.30 | AAAA AAAA |
| ATOM | 1601 | | GLU | | | | 16.997 | 21.894 | 50.835 | 1.00 30.30 | |
| MOTA | 1602 | C | | | | | | | 51.046 | 1.00 32.77 | AAAA |
| ATOM | 1603 | 0 | GLU | | | | 16.806 | 20.690 | 51.711 | | AAAA |
| MOTA | 1604 | N | LYS | | | | 17.599 | 22.690 | | 1.00 32.31 | AAAA |
| ATOM | 1605 | CA | LYS | | | | 18.101 | 22.168 | 52.974 | 1.00 32.09 | AAAA |
| MOTA | 1606 | CB | LYS | | | | 19.565 | 21.750 | 52.811 | 1.00 33.02 | AAAA |
| MOTA | 1607 | CG | LYS | | | | 19.836 | 20.847 | 51.623 | 1.00 34.95 | AAAA |
| ATOM | 1608 | CD | LYS | | | | 21.334 | 20.619 | 51.436 | 1.00 37.92 | AAAA |
| MOTA | 1609 | CE | LYS | | | | 21.655 | 19.804 | 50.169 | | AAAA |
| MOTA | 1610 | NZ | LYS | | | | 23.120 | 19.522 | 49.988 | 1.00 38.58 | AAAA |
| MOTA | 1611 | C | LYS | | | | 17.995 | 23.241 | 54.037 | 1.00 30.85 | AAAA |
| MOTA | 1612 | 0 | LYS | | | | 17.706 | 24.389 | 53.739 | 1.00 30.49 | AAAA |
| MOTA | 1613 | И | GLY | | | | 18.238 | 22.867 | 55.281 | 1.00 30.81 | AAAA |
| MOTA | 1614 | CA | GLY | | | | 18.159 | 23.831 | 56.356 | 1.00 30.86 | AAAA |
| MOTA | 1615 | C | GLY | | | | 16.991 | 23.578 | 57.280 | 1.00 30.84 | AAAA |
| ATOM | 1616 | 0 | GLY | | | | 16.828 | 24.285 | 58.272 | 1.00 31.58 | AAAA |
| MOTA | 1617 | И | PHE | | | | 16.182 | 22.570 | 56.965 | 1.00 30.54 | AAAA |
| ATOM | 1618 | CA | PHE | | | | 15.025 | 22.241 | 57.797 | 1.00 30.51 | AAAA |
| MOTA | 1619 | CB | PHE | | | | 14.061 | 21.317 21.890 | 57.058 55.787 | 1.00 29.06 1.00 27.13 | AAAA AAAA |
| ATOM | 1620 | CG | PHE | | | | 13.524 | 21.850 | 54.601 | 1.00 27.13 | AAAA |
| ATOM | 1621 | | PHE | | | | 14.222 12.307 | 22.548 | 55.779 | 1.00 26.52 | AAAA |
| ATOM | 1622 | | PHE | | | | 13.713 | 22.276 | 53.420 | 1.00 26.44 | AAAA |
| ATOM | 1623 1624 | | PHE | | | | 11.786 | 23.069 | 54.600 | 1.00 26.69 | AAAA |
| ATOM | 1625 | CZ | PHE | | | | 12.490 | 22.931 | 53.416 | 1.00 25.65 | AAAA |
| MOTA | 1626 | C | PHE | | | | 15.401 | 21.590 | 59.127 | 1.00 30.87 | AAAA |
| ATOM | 1627 | Ö | PHE | | | | 16.395 | 20.875 | 59.228 | 1.00 31.12 | AAAA |
| MOTA | 1628 | N | LEU | | | | 14.580 | 21.844 | 60.139 | 1.00 31.22 | AAAA |
| ATOM | 1629 | CA | LEU | | | | 14.782 | 21.329 | 61.489 | 1.00 31.43 | AAAA |
| MOTA | 1630 | | LEU | | | | 13.575 | 21.691 | 62.357 | 1.00 31.42 | AAAA |
| ATOM | 1631 | CG . | LEU | | | | 13.603 | 21.078 | 63.755 | 1.00 31.76 | AAAA: |
| MOTA MOTA | 1632 | | LEU | | - | | 14.894 | 21.492 | 64.457 | 1.00 32.36 | AAAA |
| MOTA | 1633 | | LEU | | | | 12.379 | 21.516 | 64.536 | 1.00 31.31 | AAAA |
| MOTA | 1634 | C | LEU | | | | 15.026 | 19.829 | 61.625 | 1.00 31.35 | AAAA |
| MOTA | 1635 | Ö | LEU | | | | 15.714 | 19.392 | 62.546 | 1.00 31.40 | AAAA |
| MOTA | 1636 | N | GLU | | | | 14.448 | 19.059 | 60.707 | 1.00 31.79 | AAAA |
| ATOM | 1637 | CA | GLU | | | | 14.509 | 17.603 | 60.706 | 1.00 32.08 | AAAA |
| ATOM | 1638 | CB | GLU | | | | 13,485 | 17.054 | 59.716 | 1.00 33.18 | AAAA |
| MOTA | 1639 | CG | GLU | | | | 12,069 | 17.651 | 59.829 | 1.00 34.20 | AAAA |
| | 1640 | CD | GLU | | | | 11.973 | 19.136 | 59.453 | 1.00 33.44 | AAAA |
| MOTA MOTA | 1641 | | GLU | | | | 10.854 | 19.675 | 59.422 | 1.00 33.32 | AAAA |
| | 1642 | | GLU | | | | 13.005 | 19.777 | 59.194 | 1.00 35.32 | AAAA |
| ATOM | 1643 | C | GLU | | | | 15.882 | 17.045 | 60.363 | 1.00 32.34 | AAAA |
| ATOM | 1644 | o | GLU | | | | 16.209 | 15.909 | 60.706 | 1.00 31.83 | AAAA |
| MOTA | | Ŋ | GLU | | | | 16.680 | 17.847 | 59.670 | 1.00 32.48 | AAAA |
| MOTA | 1645 | CA | GLU | | | | 18.017 | 17.431 | 59.287 | 1.00 31.67 | AAAA |
| MOTA | 1646 | | GLU | | | | 18.552 | 18.385 | 58.238 | 1.00 30.39 | AAAA |
| MOTA | 1647 | CB | | | | | 17.768 | 18.316 | 56.960 | 1.00 29.63 | AAAA |
| MOTA | 1648 | CG | GLU | | | | 17.768 | 19.547 | 56.121 | 1.00 30.04 | AAAA |
| ATOM | 1649 | CD | GLU | | | | | | 55.971 | 1.00 30.04 | AAAA |
| MOTA | 1650 | OE1 | GLU | H | 20/ | | 19.108 | 19.991 | JJ.7/1 | 1.00 30.31 | Anan |

| ATOM | 1651 | OE2 | GLU A | 207 | 16.947 | 20.070 | 55.604 | 1.00 30.76 | AAAA |
|-------|------|-----|--------|-------|--------|--------|--------|------------|------|
| | | | GLU A | | 18.879 | 17.433 | 60.537 | 1.00 32.04 | AAAA |
| ATOM | 1652 | | | | | 18.448 | 60.910 | 1.00 31.57 | AAAA |
| MOTA | 1653 | 0 | GLU A | | 19.472 | | | 1.00 32.57 | AAAA |
| MOTA | 1654 | N | ILE Y | 208 | 18.935 | 16.272 | 61.178 | - | |
| MOTA | 1655 | CA | ILE A | 208 | 19.674 | 16.111 | 62.408 | 1.00 33.37 | AAAA |
| MOTA | 1656 | CB | ILE A | 208 | 18.709 | 15.647 | 63.519 | 1.00 33.65 | AAAA |
| | 1657 | | ILE A | | 19.443 | 15.380 | 64.806 | 1.00 34.11 | AAAA |
| MOTA | | | | | 17.673 | 16.742 | 63.757 | 1.00 33.94 | AAAA |
| MOTA | 1658 | | ILE A | | | | 64.794 | 1.00 37.00 | AAAA |
| ATOM | 1659 | CD1 | ILE A | | 16.628 | 16.386 | | | |
| MOTA | 1660 | С | ILE A | 208 | 20.863 | 15.174 | 62.280 | 1.00 34.00 | AAAA |
| ATOM | 1661 | 0 | ILE A | 208 | 21.506 | 14.829 | 63.265 | 1.00 34.40 | AAAA |
| MOTA | 1662 | N | GLY A | 209 | 21.177 | 14.768 | 61.062 | 1.00 34.64 | AAAA |
| | 1663 | CA | GLY A | | 22.321 | 13.903 | 60.913 | 1.00 35.55 | AAAA |
| ATOM | | | GLY A | | 22.164 | 12.671 | 60.057 | 1.00 36.80 | AAAA |
| MOTA | 1664 | C | | | | 12.461 | 59.400 | 1.00 37.32 | AAAA |
| MOTA | 1665 | 0 | GLY A | | 21.148 | | | 1.00 37.78 | AAAA |
| ATOM | 1666 | N | GLU A | 210 | 23.199 | 11.836 | 60.100 | | |
| MOTA | 1667 | CA | GLU A | 210 | 23.256 | 10.621 | 59.315 | 1.00 38.04 | AAAA |
| MOTA | 1668 | CB | GLU A | 210 | 23.600 | 11.013 | 57.892 | 1.00 38.54 | AAAA |
| MOTA | 1669 | CG | GLU A | | 23.469 | 9.960 | 56.858 | 1.00 38.99 | AAAA |
| | 1670 | CD | GLU A | | 24.118 | 10.412 | 55.580 | 1.00 40.10 | AAAA |
| ATOM | | | GLU A | | 25.365 | 10.437 | 55.555 | 1.00 40.86 | AAAA |
| MOTA | 1671 | | | | | 10.767 | 54.619 | 1.00 40.41 | AAAA |
| MOTA | 1672 | OE2 | GLU A | | 23.396 | | | 1.00 37.98 | AAAA |
| MOTA | 1673 | С | GLU A | | 24.377 | 9.770 | 59.894 | | |
| ATOM | 1674 | 0 | GLU A | 210 | 25.498 | 10.244 | 60.041 | 1.00 38.52 | AAAA |
| MOTA | 1675 | N | GLY A | 211 | 24.085 | 8.517 | 60.220 | 1.00 38.02 | AAAA |
| ATOM | 1676 | CA | GLY A | | 25.116 | 7.654 | 60.770 | 1.00 38.09 | AAAA |
| | 1677 | c | GLY A | | 25.542 | 8.075 | 62.164 | 1.00 38.26 | AAAA |
| ATOM | | | GLY A | | 24.697 | 8.443 | 52.977 | 1.00 37.82 | AAAA |
| MOTA | 1678 | 0 | | | 26.848 | 8.030 | 62.434 | 1.00 38.20 | AAAA |
| MOTA | 1679 | N | LYS A | | | | 63.743 | 1.00 37.56 | AAAA |
| MOTA | 1680 | CA | LYS A | | 27.396 | 8.399 | | | AAAA |
| MOTA | 1681 | CB | LYS A | 212 | 28.921 | 8.209 | 63.766 | 1.00 38.86 | |
| ATOM | 1682 | CG | LYS A | 212 | 29.416 | 6.810 | 63.385 | 1.00 40.93 | AAAA |
| ATOM | 1683 | CD | LYS A | 212 | 29.001 | 5.746 | 64.405 | 1.00 42.04 | AAAA |
| | 1684 | CE | LYS A | | 29.251 | 4.318 | 63.891 | 1.00 42.80 | AAAA |
| MOTA | 1685 | NZ | LYS A | | 30.673 | 4.002 | 63.562 | 1.00 42.32 | AAAA |
| MOTA | | | LYS A | | 27.093 | 9.859 | 64.054 | 1.00 37.08 | AAAA |
| MOTA | 1686 | C | | | 27.075 | 10.269 | 65.218 | 1.00 36.94 | AAAA |
| ATOM | 1687 | 0 | LYS A | | | | 63.002 | 1.00 35.41 | AAAA |
| MOTA | 1688 | N | GLY A | | 26.854 | 10.636 | | 1.00 34.24 | AAAA |
| ATOM | 1689 | CA | GLY A | 213 | 26.592 | 12.054 | 63.170 | | |
| MOTA | 1690 | С | GLY A | 213 | 25.163 | 12.438 | 63.470 | 1.00 33.27 | AAAA |
| ATOM | 1691 | 0 | GLY A | 213 | 24.861 | 13.611 | 63.666 | 1.00 33.29 | AAAA |
| | 1692 | N | LYS A | | 24.280 | 11.451 | 63.512 | 1.00 31.79 | AAAA |
| MOTA | 1693 | CA | LYS A | | 22.883 | 11.710 | 63.794 | 1.00 30.47 | AAAA |
| MOTA | | | LYS A | | 22.111 | 10.396 | 63.737 | 1.00 30.35 | AAAA |
| MOTA | 1694 | CB | | | 20.676 | 10.552 | 63.280 | 1.00 30.45 | AAAA |
| MOTA | 1695 | CG | LYS A | | | 9.241 | 62.759 | 1.00 29.75 | AAAA |
| ATOM | 1696 | CD | LYS ? | | 20.141 | | | 1.00 30.19 | AAAA |
| ATOM | 1697 | CE | LYŚ A | 1 214 | 18.737 | 9.400 | 62.229 | | |
| ATOM | 1698 | NZ | LYS ? | 1 214 | 18.179 | 8.138 | 61.671 | 1.00 31.35 | AAAA |
| ATOM | 1699 | С | LYS A | 214 | 22.778 | 12.374 | 65.168 | 1.00 30.31 | AAAA |
| | 1700 | Q | LYS A | | 23.193 | 11.814 | 66.177 | 1.00 30.44 | AAAA |
| ATOM | | N | GLY A | | 22.243 | 13.590 | 65.192 | 1.00 29.95 | AAAA |
| MOTA | 1701 | | GLY 3 | | 22.128 | 14.325 | 66.437 | 1.00 29.16 | AAAA |
| ATOM | 1702 | CA | G1,1 . | 1 213 | | 15.379 | 66.582 | 1.00 28.54 | AAAA |
| MOTA | 1703 | С | GLY ? | | 23.222 | | 67.602 | 1.00 28.27 | AAAA |
| MOTA | 1704 | 0 | GLY A | | 23.306 | 16.061 | | | |
| MOTA | 1705 | Ŋ | TYR : | 4 216 | 24.063 | 15.521 | | 1.00 27.35 | AAAA |
| ATOM | 1706 | ĊA | TYR A | | 25.150 | 16.497 | 65.616 | 1.00 27.08 | AAAA |
| | 1707 | ·СВ | TYR ? | | 26.516 | 15.800 | 65.531 | 1.00 28.38 | AAAA |
| ATOM | • | CG | TYR A | | 26.786 | | 66.757 | 1.00 30.21 | AAAA |
| MOTA | 1708 | | | | | | | | AAAA |
| MOTA | 1709 | | TYR | | 26.138 | | | | AAAA |
| ATOM | 1710 | | TYR A | | 26.311 | | | | AAAA |
| ATOM | 1711 | CD2 | | | 27.619 | | | | |
| ATOM | 1712 | CE2 | TYR A | | 27.798 | 14.741 | | | AAAA |
| MCTA | 1713 | CZ | | A 216 | 27.143 | 13.528 | | | AAAA |
| | 1714 | OH | | A 216 | 27.297 | | 70.332 | | AAAA |
| ATCM | | | | A 216 | 25.055 | | | 1.00 25.40 | AAAA |
| MOTA | 1715 | C | | | | | | | AAAA |
| 2 TOM | 1716 | 0 | TYK | A 216 | 26.046 | 10.240 | | | |

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| ATOM | 1717 | N | ASN A | A 217 | 23.845 | 17.791 | 64.076 | 1.00 23.55 | AAAA |
|------|---------------|-----|--------|-------|---------|--------|--------|------------|------|
| ATOM | 1718 | CA | | A 217 | 23.549 | 18.830 | 63.119 | 1.00 21.52 | |
| ATOM | 1719 | CB | | A 217 | 23.431 | 18.282 | 61.699 | 1.00 20.64 | AAAA |
| | 1720 | CG | | A 217 | | | | | AAAA |
| ATOM | _ | | | | 23.202 | 19.386 | 60.669 | 1.00 20.29 | AAAA |
| ATOM | 1721 | | ASN A | | 22.089 | 19.888 | 60.499 | 1.00 18.03 | AAAA |
| ATOM | 1722 | | ASN I | | 24.274 | 19.790 | 60.004 | 1.00 19.95 | AAAA |
| ATOM | 1723 | С | | A 217 | 22.216 | 19.346 | 63.605 | 1.00 21.64 | AAAA |
| MOTA | 1724 | .0 | ASN I | A 217 | 21.263 | 18.576 | 63.757 | 1.00 20.34 | AAAA |
| MOTA | 1725 | N | LEU Z | A 218 | 22.165 | 20.647 | 63.873 | 1.00 22.22 | AAAA |
| ATOM | 1726 | CA | LEU 2 | A 218 | 20.960 | 21.282 | 64.388 | 1.00 22.03 | AAAA |
| MOTA | 1727 | CB | LEU | A 218 | 21.195 | 21.711 | 65.840 | 1.00 20.97 | AAAA |
| ATOM | 1728 | CG | | A 218 | 20.051 | 21.838 | 66.841 | 1.00 20.94 | AAAA |
| ATOM | 1729 | - | LEU 2 | | 20.513 | 22.744 | 67.936 | 1.00 20.31 | |
| ATOM | 1730 | | LEU | | 18.818 | 22.412 | 66.227 | 1.00 21.27 | AAAA |
| ATOM | 1731 | C | | A 218 | | | | | AAAA |
| | 1732 | | | A 218 | 20.669 | 22.513 | 63.547 | 1.00 22.70 | AAAA |
| ATOM | | 0 | | | 21.451 | 23.454 | 63.557 | 1.00 22.64 | AAAA |
| MOTA | 1733 | N | | A 219 | 19.564 | 22.491 | 62.808 | 1.00 24.00 | AAAA |
| ATOM | 1734 | CA | | A 219 | 19.166 | 23.626 | 61.990 | 1.00 25.33 | AAAA |
| MOTA | 1735 | CB | | A 219 | 18.656 | 23.190 | 60.614 | 1.00 26.94 | AAAA |
| MOTA | 1736 | CG | | A 219 | 19.737 | 22.601 | 59.749 | 1.00 26.68 | AAAA |
| MOTA | 1 7 37 | | ASN A | | 20.812 | 23.169 | 59.626 | 1.00 28.06 | AAAA |
| ATOM | 1738 | ND2 | ASN A | A 219 | 19.446 | 21.471 | 59.117 | 1.00 26.26 | AAAA |
| MOTA | 1739 | С | ASN A | 219 | 18.046 | 24.345 | 62.710 | 1.00 25.69 | AAAA |
| MOTA | 1740 | 0 | ASN A | 219 | 17.118 | 23.706 | 63.210 | 1.00 27.51 | AAAA |
| ATOM | 1741 | N | | 220 | 18.122 | 25.667 | 62.753 | 1.00 25.05 | AAAA |
| MOTA | 1742 | CA | | 220 | 17.107 | 26.457 | 63.428 | 1.00 25.87 | AAAA |
| ATOM | 1743 | CB | | 220 | 17.733 | 27.331 | 64.557 | 1.00 25.04 | AAAA |
| ATOM | 1744 | | ILE A | | 16.654 | 28.152 | 65.227 | 1.00 25.24 | AAAA |
| ATOM | 1745 | | ILE A | | 18.460 | 26.447 | 65.584 | 1.00 24.07 | |
| MOTA | 1746 | | ILE A | | 17.557 | 25.502 | 66.378 | 1.00 22.28 | AAAA |
| | 1747 | C | | 220 | 16.430 | | | 1.00 26.20 | AAAA |
| ATOM | | | ILE A | | | 27.370 | 62.414 | | AAAA |
| ATOM | 1748 | 0 | | | 16.801 | 28.534 | 62.265 | 1.00 25.35 | AAAA |
| MOTA | 1749 | N | PRO A | | 15.421 | 26.850 | 61.704 | 1.00 26.70 | AAAA |
| MOTA | 1750 | CD | | 221 . | | 25.501 | 61.778 | 1.00 27.17 | AAAA |
| MOTA | 1751 | CA | PRO A | | 14.706 | 27.640 | 60.703 | 1.00 27.67 | AAAA |
| MOTA | 1752 | CB | PRO A | | 13.771 | 26.613 | 60.064 | 1.00 26.81 | AAAA |
| MOTA | 1753 | CG | PRO A | | 14.473 | 25.293 | 60.346 | 1.00 27.36 | AAAA |
| ATOM | 1754 | ¢ | PRO A | | 13.944 | 28.763 | 61.390 | 1.00 28.61 | AAAA |
| ATOM | 1755 | 0 | PRO A | | 13.218 | 28.515 | 62.363 | 1.00 29.91 | AAAA |
| ATOM | 1756 | N | LEU A | 222 | 14.100 | 29.990 | 60.900 | 1.00 28.15 | AAAA |
| MOTA | 1757 | CA | LEU A | 222 | 13.408 | 31.117 | 61.511 | 1.00 28.48 | AAAA |
| ATOM | 1758 | CB | LEU A | 222 | 14.431 | 32.041 | 62.191 | 1.00 28.69 | AAAA |
| ATOM | 1759 | CG | LEU A | 222 | 15.187 | 31.394 | 63.371 | 1.00 28.67 | AAAA |
| MOTA | 1760 | CD1 | LEU A | 222 | 16.304 | 32.300 | 63.837 | 1.00 28.62 | AAAA |
| ATOM | 1761 | CD2 | LEU A | 222 | 14.231 | 31.106 | 64.527 | 1.00 27.65 | AAAA |
| ATOM | 1762 | С | LEU A | 222 | 12. 26 | 31.882 | 60.518 | 1.00 28.44 | AAAA |
| ATOM | 1763 | O | LEU A | | 12. ;18 | 31.958 | 59.325 | 1.00 27.90 | AAAA |
| ATOM | 1764 | N | PRO A | | . 1113 | 32.441 | 61.009 | 1.00 28.79 | AAAA |
| ATOM | 1765 | CD | PRO A | | 10.966 | 32.357 | 62.410 | 1.00 29.20 | AAAA |
| ATOM | 1766 | CA | PRO A | | 10.437 | 33.202 | 60.227 | 1.00 29.36 | AAAA |
| | | CB | PRO A | | | | | | |
| ATOM | 1767 | | | | 9.256 | 33.287 | 61.183 | 1.00 28.98 | AAAA |
| MOTA | 1768 | CG | PRO A | | 9.965 | 33.502 | 62.485 | 1.00 28.68 | AAAA |
| MOTA | 1769 | С | PRO A | | 10.890 | 34.585 | 59.753 | 1.00 30.15 | AAAA |
| MOTA | 1770 | 0 | PRO A | | 11.864 | 35.152 | 60.253 | 1.00 30.18 | AAAA |
| ATOM | 1771 | N | LYS A | | 10.150 | 35.112 | 58.781 | 1.00 30.50 | AAAA |
| MOTA | 1772 | CA | LYS A | | 10.398 | 36.422 | 58.213 | 1.00 29.92 | AAAA |
| MOTA | 1773 | CB | LYS A | | 9.491 | 36.661 | 57.008 | 1.00 30.57 | AAAA |
| MOTA | 1774 | CG | LYS A | 224 | 9.588 | 35.676 | 55.893 | 1.00 30.06 | AAAA |
| ATOM | 1775 | CD | LYS A | 224 | 8.640 | 36.087 | 54.798 | 1.00 30.91 | AAAA |
| MOTA | 1776 | CE | LYS A | 224 | 8.575 | 35.051 | 53.705 | 1.00 32.15 | AAAA |
| ATOM | 1777 | NZ | LYS A | | 7.628 | 35.476 | 52.648 | 1.00 32.75 | AAAA |
| ATOM | 1778 | c | LYS A | | 10.050 | 37.468 | 59.260 | 1.00 29.75 | AAAA |
| MOTA | 1779 | ō | LYS A | | 9.308 | 37.193 | 60.196 | 1.00 29.84 | AAAA |
| ATOM | 1780 | N | GLY A | | 10.555 | 38.678 | 59.079 | 1.00 29.39 | AAAA |
| | 1781 | CA | GLY A | | 10.353 | 39.730 | 60.031 | 1.00 29.87 | AAAA |
| MOTA | 1782 | | GLY A | | 10.809 | 39.447 | 61.415 | 1.00 29.85 | |
| ATOM | 1104 | _ | א אנוט | 223 | 10.009 | 22.44/ | 01.413 | 1.00 63.05 | AAAA |

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| ATOM | 1783 | 0 | GLY A 225 | 10.371 | 40.051 | 62.392 | 1.00 29.85 | AAAA |
|--------|-------|-----|-----------|-----------------|----------------|---------|------------|------|
| | | | | | | 61.499 | 1.00 29.50 | |
| ATOM | 1784 | N | LEU A 226 | 11.775 | 3,8.536 | | | AAAA |
| ATOM | 1785 | CA | LEU A 226 | 12.374 | 38.175 | 62.778 | 1.00 29.80 | AAAA |
| | | | | 13.513 | | 62.570 | 1.00 28.81 | AAAA |
| MOTA | 1786 | CB | LEU A 226 | | 37.170 | | | |
| MOTA | 1787 | CG | LEU A 226 | 14.097 | 36.514 | 63.820 | 1.00 27.29 | AAAA |
| | | CD1 | LEU A 226 | 13.132 | 35.452 | 64.275 | 1.00 26.06 | AAAA |
| MOTA | 1788 | | | | | | | |
| ATOM | 1789. | CD2 | LEU A 226 | 15 <i>.</i> 455 | 35.888 | 63.538 | 1.00 27.03 | AAAA |
| | 1790 | С | LEU A 226 | 12.936 | 39.428 | 63.448 | 1.00 30.68 | AAAA |
| MOTA | | | | | | | | |
| MOTA | 1791 | 0 | LEU A 226 | 13.636 | 40:217 | 62.804 | 1.00 30.57 | AAAA |
| | 1792 | N | ASN A 227 | 12.624 | 39.617 | 64.729 | 1.00 31.46 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 1793 | CA | ASN A 227 | _ 13.139 | 40.769 | 65.469 | 1.00 32.06 | AAAA |
| | 1794 | CB | ASN A 227 | 12.012 | 41.507 | 66.217 | 1.00 31.74 | AAAA |
| MOTA | | | | | | | | |
| MOTA | 1795 | CG | ASN A 227 | 11.291 | 40.630 | 67.234 | 1.00 32.07 | AAAA |
| MOTA | 1796 | ODI | ASN A 227 | 11.914 | 40.017 | 68.104 | 1.00 31.61 | AAAA |
| | | | | | | | 1.00 31.59 | |
| MOTA | 1797 | NDZ | ASN A 227 | 9.962 | 40.592 | 67.141 | | AAAA |
| MOTA | 1798 | С | ASN A 227 | 14.225 | 40.334 | 66.444- | 1.00 32.45 | AAAA |
| | | | | | | 66.688 | 1.00 32.78 | |
| ATOM | 1799 | 0 | ASN A 227 | . 14.413 | 39.140 | | | AAAA |
| MOTA | 1800 | N | ASP A 228 | 14.943 | 41.297 | 67.002 | 1.00 33.32 | AAAA |
| | | | | · · | 40.976 | 67.928 | 1.00 34.75 | AAAA |
| MOTA | 1801 | CA | ASP A 228 | | | | | |
| ATOM | 1802 | CB | ASP A 228 | 16.508 | 42.233 | 68.654 | 1.00 36.77 | AAAA |
| | | ĊG | ASP A 228 | | 43.238 | 67.714 | 1.00 37.28 | AAAA |
| MOTA | 1803 | | | | | | | |
| MOTA | 1804 | OD1 | ASP A 228 | 17.662 | 42.816 | 66.652 | 1.00 37.78 | AAAA |
| | 1805 | 002 | ASP A 228 | 17.180 | 44.443 | 68.054 | 1.00 37.21 | AAAA |
| ATOM | | | | | | | | |
| ATOM | 1806 | С | ASP A 228 | 15.707 | 39.892 | 68.964 | 1.00 34.93 | AAAA |
| MOTA | 1807 | 0 | ASP A 228 | 16.448 | 38.919 | 69.056 | 1.00 36.92 | AAAA |
| | | • | | | | 69.741 | 1.00 33.90 | AAAA |
| ATOM | 1808 | N | ASN A 229 | 14.635 | 40.054 | | | |
| MOTA | 1809 | ÇA | ASN A 229 | 14.268 | 39.079 | 70.775 | 1.00 33.01 | AAAA |
| | | | ASN A 229 | | 39.481 | 71.455 | 1.00 33.79 | AAAA |
| ATOM | 1810 | CB | | | | | | |
| MOTA | 1811 | CG | ASN A 229 | 13.131 | 40.663 | 72.369 | 1.00 34.04 | AAAA |
| | | זמס | ASN A 229 | 13.783 | 40.564 | 73.405 | 1.00 34.25 | AAAA |
| ATOM - | | | | | | | | |
| ATOM | 1813 | ND2 | ASN A 229 | 12.550 | 41.797 | 71.988 | 1.00 34.05 | AAAA |
| ATOM | 1814 | С | ASN A 229 | 14.114 | 37.656 | 70.276 | 1.00 32.98 | AAAA |
| | | | | | | | 1.00 32.77 | AAAA |
| ATOM | 1815 | 0 | ASN A 229 | | 36.697 | • | | |
| ATOM | 1816 | N | GLU A 230 | 13.496 | 37.523 | 69.108 | 1.00 32.02 | AAAA |
| | | • | GLU A 230 | | 36.227 | 68.516 | 1.00 30.72 | AAAA |
| MOTA | 1817 | CA | | | | | | |
| MOTA | 1818 | CB | GLU A 230 | 12.399 | 36.375 | 67.272 | 1.00 31.38 | AAAA |
| | 1819 | CG | GLU A 230 | 11.006 | 36.896 | 67.583 | 1.00 31.02 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 1820 | CD | GLU A 230 | 10.175 | 37.187 | 66.350 | 1.00 31.52 | AAAA |
| ATOM | 1821 | OE1 | GLU A 230 | 10.644 | 37.970 | 65.497 | 1.00 31.89 | AAAA |
| | | | | | | | 1.00 31.04 | AAAA |
| MOTA | 1822 | QE2 | GLU A 230 | 9.047 | 36.655 | 66.241 | | |
| MOTA | 1823 | С | GLU A 230 | 14.628 | 35.622 | 68.180 | 1.00 30.79 | AAAA |
| | | | GLU A 230 | | 34.465 | 68.512 | 1.00 31.05 | AAAA |
| MOTA | 1824 | 0 | | | | | | |
| ATOM | 1825 | N | PHE A 231 | 15.490 | 36.412 | 67.553 | 1.00 30.05 | AAAA |
| | 1826 | CA | PHE A 231 | 16.811 | 35.920 | 67.191 | 1.00 28.94 | AAAA |
| MOTA | | | | | | | 1.00 29.33 | AAAA |
| ATOM | 1827 | CB | PHE A 231 | 17.632 | 37.015 | 66.528 | | |
| ATOM | 1828 | CG | PHE A 231 | 18.949 | 36.537 | 65.972 | 1.00 28.79 | AAAA |
| | | | | | 35.585 | 64.957 | 1.00 28.93 | AAAA |
| MOTA | 1829 | | PHE A 231 | | | | | |
| ATOM | 1830 | CD2 | PHE A 231 | 20.152 | 37.067 | 66.436 | 1.00 28.55 | AAAA |
| | 1831 | CE1 | PHE A 231 | 20.195 | 35.160 | 64.397 | 1.00 28.32 | AAAA |
| MOTA | | | | | | | | |
| ATOM | 1832 | CE2 | PHE A 231 | | 36.657 | 65.888 | 1.00 28.97 | AAAA |
| ATOM | 1833 | CZ | PHE A 231 | 21.397 | 35.695 | 64.860 | 1.00 28.81 | AAAA |
| | | | | 17 FEO | | 68.413 | 1.00 28.25 | AAAA |
| MOTA | 1834 | С | PHE A 231 | | 35.443 | | | |
| ATOM | 1835 | 0 | PHE A 231 | 17.999 | 34.302 | 68.485 | 1.00 27.97 | AAAA |
| | | | | 17.691 | 36.329 | -69.384 | 1.00 27.93 | AAAA |
| MOTA | 1836 | N | LEU A 232 | | | | | |
| MOTA | 1837 | CA | LEU A 232 | 18.425 | 36.003 | 70.590 | 1.00 27.93 | AAAA |
| | | CB | LEU A 232 | 18.521 | 37.234 | 71.484 | 1.00 28.16 | AAAA |
| MOTA | 1838 | | | | | | | |
| ATOM | 1839 | CG | LEU A 232 | 19.220 | 38.37 <i>9</i> | 70.747 | 1.00 27.96 | AAAA |
| | 1840 | | LEU A 232 | 19.203 | 39.629 | 71.587 | 1.00 27.57 | AAAA |
| ATOM | | | | | | | | AAAA |
| MOTA | 1841 | CD2 | LEU A 232 | 20.639 | 37.955 | 70.387 | 1.00 27.76 | |
| | 1842 | С | LEU A 232 | 17.815 | 34.851 | 71.340 | 1.00 27.95 | AAAA |
| ATOM | | | | | | | 1.00 27.92 | AAAA |
| ATOM | 1843 | 0 | LEU A 232 | | 34.061 | 71.941 | | |
| ATCM | 1844 | N | PHE A 233 | 16.495 | 34.758 | 71.298 | 1.00 28.81 | AAAA |
| | | | | | 33.685 | 71.972 | 1.00 30.27 | AAAA |
| MOTE | 1845 | CA | PHE A 233 | 15.786 | | | | |
| ATOM | 1846 | CB | PHE A 233 | 14.278 | 33.837 | 71.745 | 1.00 31.51 | AAAA |
| | | | PHE A 233 | 13.465 | 32.710 | 72.308 | 1.00 32.38 | AAAA |
| ATOM | 1847 | CG | | | | | | |
| ATOM | 1848 | CD1 | PHE A 233 | 13.257 | 32.599 | 73.677 | 1.00 33.66 | AAAA |
| | - | | | | | - | | _ |

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| MOTA | 1849 | CD2 | PHE A | 233 | 12.928 | 31.741 | 71.467 | 1.00 | 33.51 | AAAA |
|--------|--------|-----|---------|-------|--------|--------|---------|------|-------------------|--------|
| ATOM | 1850 | | PHE A | | 12.518 | 31.537 | 74.201 | | 35,10 | |
| ATOM | 1851 | | PHE A | | | | | | | AAAA |
| | | | | | 12.193 | 30.677 | 71.975 | | 34.21 | AAAA |
| ATOM | 1852 | CZ | PHE A | | 11.986 | 30.572 | 73.344 | | 35.23 | AAAA |
| MOTA | 1853 | С | PHE A | | 16.219 | 32.301 | 71.483 | 1.00 | 30.55 | AAAA |
| - MOTA | 1854 | 0 | PHE A | 233 | 16.438 | 31.391 | 72.280 | 1.00 | 30.65 | AAAA |
| ATOM | 1855 | N | ALA A | 234 | 16.317 | 32.151 | 70.165 | | 30.21 | AAAA |
| ATOM | 1856 | CA | ALA A | | 16.698 | 30.892 | 69.549 | | 28.97 | |
| | 1857 | CB | | | 16.398 | | | | | AAAA |
| ATOM | | | ALA A | | | 30.942 | | | 30.40 | AAAA |
| MOTA | 1858 | С | ALA A | | 18.169 | 30.571 | 69.761 | 1.00 | 28.27 | AAAA |
| MOTA | 1859 | 0 | ALA A | 234 | 18.564 | 29.401 | 69.830 | 1.00 | 26.6 9 | AAAA |
| MOTA | 1860 | N | LEU A | 235 | 18.978 | 31.614 | 69.855 | 1.00 | 27.56 | AAAA |
| MOTA | 1861 | CA | LEU A | 235 · | 20.402 | 31.427 | 70.055- | 1.00 | 29.17 | AAAA |
| MOTA | 1862 | CB | LEU A | | 21.126 | 32.767 | 69.989 | | 29.04 | AAAA |
| ATOM | 1863 | CG | LEU A | | 22.527 | 32.757 | 69.378 | | | |
| | | | | | | | | | 28.54 | AAAA |
| MOTA | 1864 | | LEU A | | 23.350 | 33.837 | 70.058 | | 27.05 | - AAAA |
| MOTA | 1865 | | LEU A | | 23.182 | 31.408 | 69.558 | 1.00 | 27.21 | AAAA |
| MOTA | 1866 | С | LEU A | 235 . | 20.637 | 30.799 | 71.429 | 1.00 | 30.99 | AAAA |
| MOTA | 1867 | Ο. | LEU A | 235 | 21.159 | 29.697 | 71.547 | 1.00 | 31.65 | AAAA |
| MOTA | 1868 | N | GLU A | 236 | 20.242 | 31.514 | 72.471 | 1.00 | 31.88 | AAAA |
| ATOM | 1869 | CA | GLU A | | 20.409 | 31.042 | 73.838 | | 32.99 | AAAA |
| ATOM | 1870 | СВ | GLU A | | 19.689 | 31.990 | 74.790 | | | |
| | | | | | | | | | 34.63 | AAAA |
| ATOM | 1871 | CG | GLU A | | 19.980 | 33.449 | 74.531 | | 36.79 | AAAA |
| MOTA | 1872 | CD | GLU A 2 | | 19.044 | 34.360 | 75.294 | | 38.99 | AAAA |
| ATOM | . 1873 | | GLU A | | 17.803 | 34.303 | 75.070 | 1.00 | 39.03 | AAAA |
| ATOM | 1874 | OE2 | GLU A 2 | 236 | 19.559 | 35.132 | 76.126 | 1.00 | 41.56 | AAAA |
| ATOM | 1875 | С | GLU A 2 | 236 | 19.806 | 29.656 | 73.982 | 1.00 | 32.94 | AAAA |
| ATOM | 1876 | 0 | GLU A 2 | 236 | 20.379 | 28.753 | 74.595 | | 31.76 | AAAA |
| ATOM | 1877 | N | LYS A 2 | | 18.631 | 29.503 | 73.399 | | 32.83 | AAAA |
| ATOM | 1878 | CA | LYS A 2 | | 17.906 | 28.256 | 73.471 | | 33.59 | |
| | | | | | | | | | | AAAA |
| ATOM | 1879 | CB | LYS A 2 | | 16.504 | 28.506 | 72.942 | | 35.00 | AAAA |
| ATOM | 1880 | CG | LYS A 2 | | 15.516 | 27.436 | 73.213 | | 36.69 | AAAA |
| ATOM | 1881 | CD | LYS A 2 | 237 | 14.310 | 28.008 | 73.940 | 1.00 | 38.53 | AAAA |
| MOTA | 1882 | CE | LYS A 2 | 237 | 14.636 | 28.331 | 75.392 | 1.00 | 39.27 | AAAA |
| ATOM | 1883 | NZ | LYS A 2 | 237 | 13.398 | 28.531 | 76.204 | 1.00 | 39.42 | AAAA |
| ATOM | 1884 | С | LYS A 2 | 237 | 18.619 | 27.129 | 72.707 | 1.00 | 33.14 | AAAA |
| ATOM | 1885 | 0 | LYS A 2 | | 18.850 | 26.051 | 73.260 | | 33.29 | AAAA |
| ATOM | 1886 | N | SER A 2 | | 18.985 | 27.374 | 71.452 | | 32.13 | |
| | 1887 | CA | | | | | | | | AAAA |
| MOTA | | | SER A 2 | | 19.671 | 26.345 | 70.685 | | 31.25 | AAAA |
| MOTA | 1888 | CB | SER A 2 | | 19.740 | 26.717 | 69.194 | | 30.52 | AĄAA |
| MOTA | 1889 | OG | SER A 2 | | 20.544 | 27.851 | 68.970 | 1.00 | 29.95 | AAAA |
| MOTA | 1890 | С | SER A 2 | 238 | 21.075 | 26.064 | 71.236 | 1.00 | 31.21 | AAAA |
| MOTA | 1891 | 0 | SER A 2 | 238 | 21.556 | 24.929 | 71.169 | 1.00 | 30.06 | AAAA |
| MOTA | 1892 | N | LEU A 2 | 239 | 21.740 | 27.077 | 71.782 | 1.00 | 31.71 | AAAA |
| ATOM | 1893 | CA | LEU A 2 | 239 | 23.070 | 26.842 | 72.351 | | 33.47 | AAAA |
| MOTA | 1894 | CB | LEU A 2 | | 23.698 | 28.13C | 72.900 | | 31.25 | AAAA |
| ATOM | 1895 | ĊĠ | LEU A 2 | | 23.988 | 29.30 | 71.977 | | | |
| | | | | | | | | | 29.80 | AAAA |
| MOTA | 1896 | | LEU A 2 | | 24.589 | 30.414 | 72.787 | | 29.05 | AAAA |
| ATOM | 1897 | | LEU A 2 | _ | 24.919 | 28.903 | 70.872 | 1.00 | 29.36 | AAAA |
| MOTA | 1898 | C | LEU A 2 | 139 | 22.933 | 25.839 | 73.502 | 1.00 | 35.41 | AAAA |
| MOTA | 1899 | 0 | LEU A 2 | 239 | 23.812 | 25.012 | 73.735 | 1.00 | 36.25 | AAAA |
| ATOM | 1900 | N | GLU A 2 | 40 | 21.816 | 25.906 | 74.213 | 1.00 | 37.34 | AAAA |
| ATOM | 1901 | CA | GLU A 2 | | 21.594 | 25.005 | 75.331 | | 39.39 | AAAA |
| ATOM | 1902 | CB | GLU A 2 | | 20.281 | 25.361 | 76.017 | | 41.90 | |
| | | | | | | | | | | AAAA |
| ATOM | 1903 | CG | GLU A 2 | | 20.040 | 24.610 | 77.308 | | 45.52 | AAAA |
| MOTA | 1904 | CD | GLU A 2 | | 19.665 | 25.552 | 78.432 | | 47.80 | AAAA |
| ATOM | 1905 | | GLU A 2 | | 18.670 | 26.295 | 78.274 | 1.00 | 49.70 | AAAA |
| MOTA | 1906 | OE2 | GLU A 2 | 40 | 20.364 | 25.559 | 79.469 | 1.00 | 48.04 | AAAA. |
| ATOM | 1907 | С | GLU A 2 | 40 | 21.583 | 23.555 | 74.875 | | 38.80 | AAAA |
| MOTA | 1908 | õ | GLU A 2 | | 22.224 | 22.700 | | | 37.85 | AAAA |
| ATOM | 1909 | N | ILE A 2 | | 20.847 | 23.293 | 73.804 | | 39.66 | AAAA |
| | | | | | | _ | | | | |
| ATOM | 1910 | CA | ILE A 2 | | 20.751 | 21.955 | 73.223 | | 40.81 | AAAA |
| ATOM | 1911 | CB | ILE A 2 | | 19.912 | 21.994 | 71.917 | | 41.10 | AAAA |
| MOTA | 1912 | | ILE A 2 | | 19.850 | 20.621 | 71.287 | | 40.88 | AAAA |
| ATOM | 1913 | CG1 | ILE A 2 | 41 | 18.502 | 22.514 | 72.220 | 1.00 | 41.45 | AAAA |
| MOTA | 1914 | CD1 | ILE A 2 | 41 | 17.641 | 22.745 | 70.992 | 1.00 | 41.14 | AAAA |
| _ | | | | | | | _ | | | |

| | | | | | | • | | | _ | | |
|--------|------|-----|-------|-----|-------|---|--------|--------|--------|------------|--------|
| ATOM | 1915 | С | ILE | Α | 241 | | 22.159 | 21.424 | 72.893 | 1.00 41.66 | AAAA |
| ATOM | 1916 | Ō | ILE | | | | 22.445 | 20.229 | 73.045 | 1.00 42.10 | AAAA |
| | | И | VAL | | | | 23.026 | 22.324 | 72.432 | 1.00 41.42 | AAAA |
| ATOM | 1917 | | | | | | 24.394 | 21.977 | 72.076 | 1.00 41.23 | AAAA |
| MOTA | 1918 | CA | VAL | | | | | | 71.351 | 1.00 40.40 | AAAA |
| MOTA | 1919 | CB | VAL | | | | 25.089 | 23.146 | | | |
| MOTA | 1920 | CG1 | VAL | A | 242 | | 26.556 | 22.850 | 71.171 | 1.00 39.25 | AAAA |
| ATOM | 1921 | CG2 | VAL | A | 242 | | 24.438 | 23.384 | 70.004 | 1.00 39.79 | AAAA |
| MOTA | 1922 | C | VAL | | | | 25.228 | 21.604 | 73.298 | 1.00 42.67 | AAAA |
| | | ō | VAL | | | | 25.882 | 20.562 | 73.316 | 1.00 41.83 | AAAA |
| MOTA | 1923 | | | | | | | 22.456 | 74.318 | 1.00 44.41 | AAAA |
| MOTA | 1924 | N | LYS | | | | 25.198 | | | 1.00 46.51 | AAAA |
| ATOM | 1925 | CA | LYS | A | 243 | | 25.972 | 22.215 | 75.523 | | |
| ATOM | 1926 | CB | LYS | Α | 243 | | 25.797 | 23.363 | 76.522 | 1.00 47.29 | AAAA |
| ATOM | 1927 | CG | LYS | Α | 243 | | 26.820 | 23.312 | 77.664 | 1.00 48.40 | AAAA · |
| ATOM | 1928 | CD | LYS | | | | 26.479 | 24.248 | 78.823 | 1.00 48.88 | AAAA |
| • | | CE | LYS | | | | 26.355 | 25.691 | 78.380 | 1.00 49.62 | AAAA |
| MOTA | 1929 | | | | | | | 26.576 | 79.505 | 1.00 50.11 | AAAA |
| MOTA | 1930 | NZ | LYS | | | | 25.926 | | | 1.00 47.59 | AAAA |
| MOTA | 1931 | С | LYS | | | | 25.639 | 20.891 | 76.209 | | |
| MOTA | 1932 | 0 | LYS | Α | 243 | | 26.537 | 20.216 | 76.711 | 1.00 48.17 | AAAA |
| MOTA | 1933 | N | GLU | A | 244 | | 24.362 | 20.517 | 76.237 | 1.00 48.86 | AAAA |
| ATOM | 1934 | CA | GLU | A | 244 | • | 23.957 | 19.262 | 76.877 | 1.00 50.82 | AAAA |
| | | CB | | | 244 | | 22.432 | 19.208 | 77.103 | 1.00 52.08 | AAAA |
| MOTA | 1935 | | | | | | 21.818 | 20.405 | 77.829 | 1.00 53.82 | AAAA |
| ATOM | 1936 | CG | GLU | | | | | | 78.230 | 1.00 54.49 | AAAA |
| MOTA | 1937 | CD | | | 244 | | 20.359 | 20.174 | | | AAAA |
| MOTA | 1938 | OEl | GLU | A | 244 | | 19.666 | 21.158 | 78.595 | 1.00 55.15 | |
| ATOM | 1939 | OE2 | GLU | A | 244 | | 19.912 | 19.006 | 78.200 | 1.00 54.98 | AAAA |
| MOTA | 1940 | С | GLU | Α | 244 | | 24.338 | 18.046 | 76.033 | 1.00 51.06 | AAAA |
| ATOM | 1941 | ō | | | 244 | | 24.206 | 16.905 | 76.477 | 1.00 51.68 | AAAA |
| | | N | | | 245 | | 24.810 | 18.292 | 74.820 | 1.00 51.12 | AAAA |
| MOTA | 1942 | | | | 245 | • | 25.149 | 17.212 | 73.904 | 1.00 50.08 | AAAA |
| MOTA | 1943 | CA | | | | | | | 72.677 | 1.00 50.22 | AAAA |
| ATOM | 1944 | СB | | | 245 | | 24.217 | 17.263 | | 1.00 51.07 | AAAA |
| ATOM | 1945 | CG1 | VAL | A | 245 | | 24.615 | 16.217 | 71.651 | | |
| ATOM | 1946 | CG2 | VAL | A | 245 | | 22.794 | 17.049 | 73.118 | 1.00 50.79 | AAAA |
| ATOM | 1947 | С | VAL | A | 245 | | 26.578 | 17.254 | 73.397 | 1.00 49.43 | AAAA |
| ATOM | 1948 | Ō | | | 245 | | 27.101 | 16.250 | 72.917 | 1.00 48.65 | AAAA |
| | | N | | | 246 | | 27.220 | 18.408 | 73.522 | 1.00 48.65 | AAAA |
| ATOM | 1949 | | | | 246 | | 28.556 | 18.552 | 72.982 | 1.00 47.97 | AAAA |
| MOTA | 1950 | CA | | | | | | | 71.607 | 1.00 46.45 | AAAA |
| MOTA | 1951 | CB | | | 246 | | 28.420 | 19.212 | | 1.00 45.35 | AAAA |
| ATOM | 1952 | CG | | | 246 | | 29.553 | 18.932 | 70.671 | | |
| MOTA | 1953 | CD1 | PHE | Α | 246 | | 29.841 | 17.629 | 70.280 | 1.00 44.13 | AAAA |
| ATOM | 1954 | CD2 | PHE | A | 246 | | 30.291 | 19.972 | 70.124 | 1.00 44.40 | AAAA |
| ATOM | 1955 | | PHE | | | | 30.840 | 17.370 | 69.356 | 1.00 43.95 | AAAA |
| | 1956 | | PHE | | | | 31.292 | 19.721 | 69.197 | 1.00 43.47 | AAAA |
| MOTA | | | | | 246 | | 31.566 | | 68.811 | 1.00 44.05 | AAAA |
| ATOM | 1957 | CZ | | | | | 29.481 | 19.383 | 73.860 | 1.00 48.60 | AAAA |
| MOTA | 1958 | С | | | 246 | | | | 74.239 | 1.00 49.59 | AAAA |
| MOTA | 1959 | 0 | | | 246 | | 29.132 | 20.501 | | | AAAA |
| ATOM | 1960 | N | GLU | Α | 247 | | 30.647 | | 74.198 | 1.00 48.69 | |
| ATOM . | 1961 | CA | GLU | A | 247 | | 31.644 | 19.578 | 74.977 | 1.00 49.45 | AAAA |
| ATOM | 1962 | CB | GLU | A | 247 | | 32.174 | 18.768 | 76.178 | 1.00 51.91 | AAAA |
| | 1963 | CG | | | 247 | | 31.257 | | 77.398 | 1.00 54.39 | AAAA |
| MOTA | | | | | 247 | | 29.986 | | 77.146 | 1.00 57.34 | AAAA |
| MOTA | 1964 | CD | | | | | | | | | AAAA |
| ATOM | 1965 | OEI | GLU | | 247 | | 29.100 | | 77.702 | 1.00 57.95 | AAAA |
| MOTA | 1966 | OE2 | GLU | y | . 247 | | 29.877 | | | 1.00 37.33 | |
| MOTA | 1967 | С | GLU | ٦, | 247 | | 32.807 | 19.903 | 74.024 | | AAAA |
| ATOM | 1968 | 0 | | | 247 | | 33.742 | 19.119 | 73.872 | | AAAA |
| | 1969 | N | | | 248 | | 32.748 | | 73.371 | 1.00 46.25 | AAAA |
| ATOM | | | | | 248 | | 31.651 | _ | 73.543 | 1.00 46.49 | AAAA |
| ATOM | 1970 | CD | | | | | | | 72.411 | | AAAA |
| MOTA | 1971 | CA | | | 248 | | 33.710 | | 72.017 | | AAAA |
| MOTA | 1972 | CB | | | 248 | | 33.063 | | | | |
| ATOM | 1973 | CG | PRC | A | 248 | | 31.604 | | 72.178 | | AAAA |
| ATOM | 1974 | c | PRC | Α (| 248 | | 35.155 | 21.814 | 72.880 | | AAAA |
| ATOM | 1975 | ō | | | 248 | | 35.401 | | | | AAAA |
| | | | | | 249 | | 36.100 | | 72.059 | | AAAA |
| ATOM | 1976 | N | | | | | | | 72.340 | | AAAA |
| MOTA | 1977 | CA | بالذي | | 249 | | 37.522 | | | | AAAA |
| MOTA | 1978 | CB | GLU | 1 2 | 249 | | 38.344 | | | | |
| ATOM | 1979 | CG | GLU | i A | 249 | | 37.960 | | | | AAAA |
| ATOM | 1980 | CD | GLU | 7 7 | 249 | | 38.825 | 18.007 | 71.241 | 1.00 40.96 | AAAA |
| ALOH. | 2200 | | | | | | | | - | | • |

| » movi | 1001 | 05. | | 240 | 38.871 | 10 017 | | | |
|--------|------|------|-----------|------------|--------|--------|--------|------------|------|
| MOTA | 1981 | | L GLU A | | | 18.017 | 69.996 | 1.00 41.55 | AAAA |
| MOTA | 1982 | OE2 | | | 39.462 | 17.187 | 71.926 | 1.00 42.49 | AAAA |
| ATOM | 1983 | С | GLU A | 249 | 37.840 | 22.873 | 71.718 | 1.00 38.81 | AAAA |
| MOTA | 1984 | 0 | GLU A | 249 | 38.715 | 23.617 | 72.181 | 1.00 38.27 | AAAA |
| ATOM | 1985 | N | VAL A | 250 | 37.109 | 23.160 | 70.644 | 1.00 36.60 | AAAA |
| ATOM | 1986 | CA | VAL A | | 37.242 | 24.402 | 69.890 | 1.00 34.20 | |
| | | | VAL A | - | | | | | AAAA |
| ATOM | 1987 | CB | | | 38.379 | 24.321 | 68.862 | 1.00 33.73 | AAAA |
| MOTA | 1988 | | L VAL A 2 | | 38.085 | 23.209 | 67.864 | 1.00 33.26 | AAAA |
| MOTA | 1989 | CG2 | VAL A. | 250 | 38.546 | 25.678 | 68.153 | 1.00 33.75 | AAAA |
| ATOM | 1990 | С | VAL A | 250 | 35.945 | 24.617 | 69.130 | 1.00 31.98 | AAAA |
| MOTA | 1991 | 0 | VAL A | | 35.205 | 23.658 | 68.904 | 1.00 32.36 | AAAA |
| MOTA | 1992 | N | TYR A | | 35.657 | | 68.760 | _ | |
| | | | | | | 25.863 | | 1.00 28.65 | AAAA |
| MOTA | 1993 | CA | TYR A | | 34.449 | 26.150 | 67.991 | 1.00 26.49 | AAAA |
| MOTA | 1994 | CB | TYR A 2 | | 33.241 | 26.442 | 68.906 | 1.00 24.32 | AAAA |
| ATOM | 1995 | CG | TYR A | 251 | 33.193 | 27.853 | 69.465 | 1.00 22.96 | AAAA |
| ATOM | 1996 | CD | L TYR A | 251 | 32.771 | 28.931 | 68.668 | 1.00 22.21 | AAAA |
| ATOM | 1997 | CE1 | TYR A 2 | 251 | 32.791 | 30.234 | 69.151 | 1.00 21.29 | AAAA |
| MOTA | 1998 | CD2 | | | 33.628 | 28.124 | 70.771 | 1.00 21.47 | |
| | | CE2 | | | | | | | AAAA |
| MOTA | 1999 | | | | 33.651 | 29.425 | 71.265 | 1.00 20.80 | AAAA |
| MOTA | 2000 | CZ | TYR A | | 33.237 | 30.475 | 70.449 | 1.00 20.77 | AAAA |
| MOTA | 2001 | OH | TYR A 2 | 251 | 33.309 | 31.768 | 70.913 | 1.00 21.41 | AAAA |
| ATOM | 2002 | С | TYR A 2 | 251 | 34.691 | 27.345 | 67.092 | 1.00 24.59 | AAAA |
| ATOM | 2003 | 0 | TYR A 2 | 251 | 35.504 | 28,216 | 67.410 | 1.00 25.87 | AAAA |
| ATOM | 2004 | N | LEU A 2 | | 33.984 | 27.374 | 65.970 | 1.00 22.49 | AAAA |
| ATOM | 2005 | CA | LEU A 2 | | 34.082 | • | 65.045 | 1.00 20.96 | |
| | | | | | | 28.482 | | | AAAA |
| ATOM | 2006 | CB | LEU A 2 | | 34.523 | | 63.657 | 1.00 21.31 | |
| MOTA | 2007 | CG | LEU A 2 | | 35.940 | 27.472 | 63.556 | 1.00 21.03 | AAAA |
| MOTA | 2008 | | LEU A 2 | | 35.947 | 26.028 | 63.977 | 1.00 22.16 | AAAA |
| MOTA | 2009 | CD2 | LEU A 2 | !52 | 36.440 | 27.594 | 62.143 | 1.00 22.13 | AAAA |
| MOTA | 2010 | С | LEU A 2 | 252 | 32.731 | 29.159 | 64.959 | 1.00 19.60 | AAAA |
| MOTA | 2011 | 0 | LEU A 2 | 252 | 31.689 | 28.523 | | 1.00 19.95 | AAAA |
| MOTA | 2012 | N | LEU A 2 | | 32.748 | 30.461 | 64.756 | 1.00 17.95 | AAAA |
| ATOM | 2013 | CA | LEU A 2 | | 31.521 | | 64.675 | | |
| | | | | | | 31.222 | | 1.00 17.33 | AAAA |
| MOTA | 2014 | CB | LEU A 2 | | 31.441 | 32.142 | 65.900 | 1.00 16.31 | AAAA |
| MOTA | 2015 | CG | LEU A 2 | | 30.266 | 33.070 | 66.153 | 1.00 15.81 | AAAA |
| MOTA | 2016 | | LEU A 2 | | 28.990 | 32.267 | 66.377 | 1.00 14.74 | AAAA |
| ATOM | 2017 | CD2 | LEU A 2 | :53 | 30.602 | 33.925 | 67.368 | 1.00 15.83 | AAAA |
| MOTA | 2018 | С | LEU A 2 | 53 | 31.564 | 32.035 | 63.386 | 1.00 16.60 | AAAA |
| ATOM | 2019 | 0 | LEU A 2 | | 32.548 | 32.722 | 63.132 | 1.00 16.40 | AAAA |
| ATOM | 2020 | N | GLN A 2 | | 30.526 | 31.936 | 62.557 | 1.00 15.88 | AAAA |
| ATOM | 2021 | CA | GLN A 2 | | 30.507 | | | 1.00 16.27 | |
| | | | | | | 32.716 | 61.328 | | AAAA |
| ATOM | 2022 | CB | GLN A 2 | | 30.045 | 31.881 | 60.121 | 1.00 15.88 | AAAA |
| ATOM | 2023 | CG | GLN A 2 | | 28.587 | 32.048 | 59.734 | 1.00 18.52 | |
| ATOM | 2024 | CD | GLN A 2 | | 28.380 | 32.935 | 58.519 | 1.00 17.54 | AAAA |
| ATOM | 2025 | OE1 | GLN A 2 | 54 | 28.714 | 32.572 | 57.391 | 1.00 15.89 | AAAA |
| MOTA | 2026 | NE2 | GLN A 2 | 54 | 27.828 | 34.103 | 58.750 | 1 00 18.49 | AAAA |
| ATOM | 2027 | С | GLN A 2 | 54 | 29.527 | 33.825 | 61.650 | 1 00 16.91 | AAAA |
| ATOM | 2028 | ō | GLN A 2 | | 28.450 | 33.571 | 62.198 | 1 00 17.41 | AAAA |
| | 2029 | N | LEU A 2 | | 29.911 | 35.053 | 61.319 | 1.00 16.68 | |
| ATOM | | | LEU A 2 | | | | | | AAAA |
| ATOM | 2030 | CA | | | 29.102 | 36.215 | 61.619 | 1.00 16.42 | AAAA |
| MOTA | 2031 | CB | LEU A 2 | | 29.861 | 37.080 | 52.616 | 1.00 14.93 | AAAA |
| MOTA | 2032 | · CG | LEU A 2 | | 30.269 | 36.301 | 63.860 | 1.00 13.90 | AAAA |
| ATOM | 2033 | CD1 | LEU A 2 | 55 | 31.494 | 36.924 | 64.515 | 1.00 12.24 | AAAA |
| ATOM | 2034 | CD2 | LEU A 2 | 5 5 | 29.083 | 36.202 | 64.774 | 1.00 12.80 | AAAA |
| ATOM | 2035 | С | LEU A 2 | | 28.699 | 37.048 | 60.404 | 1.00 18.32 | AAAA |
| | 2036 | ō | LEU A 2 | | 29.170 | | 60.216 | 1.00 17.59 | |
| ATOM | | | | | | 38.177 | | | AAAA |
| MOTA | 2037 | N | GLY A 2 | | 27.813 | 36.482 | 59.588 | 1.00 19.75 | AAAA |
| MOTA | 2038 | CA | GLY A 2 | | 27.322 | 37.188 | 58.422 | 1.00 20.77 | AAAA |
| ATOM | 2039 | С | GLY A 2 | 56 | 26.422 | 38.302 | 58.927 | 1.00 21.73 | AAAA |
| MOTA | 2040 | 0 | GLY A 2 | 56 | 25.642 | 30.096 | 59.857 | 1.00 21.38 | AAAA |
| ATOM | 2041 | N | THR A 2 | | 26.528 | 39.485 | 58.325 | 1.00 22.82 | AAAA |
| ATOM | 2042 | CA | THR A 2 | | 25.721 | 40.622 | 58.746 | 1.00 23.85 | AAAA |
| | 2042 | CB | THR A 2 | | 26.460 | | | 1.00 23.99 | |
| ATOM | | | | | | 41.968 | 58.549 | | AAAA |
| ATOM | 2044 | | THR A 2 | | 26.729 | 42.169 | 57.153 | 1.00 25.54 | AAAA |
| MOTA | 2045 | CG2 | THR A 2 | | 27.780 | 41.985 | 59.329 | 1.00 24.07 | AAAA |
| ATOM | 2046 | С | THR A 2 | 57 | 24.438 | 40.691 | 57.948 | 1.00 24.97 | AAAA |

| MOTA | 2047 | 0 | THR | Δ | 257 | 23.692 | 41.672 | 58.048 | 1.00 25.84 | AAAA |
|--------|-------|-----|-----|---|-------|--------|--------|---------|------------|--------|
| | | | ASP | | | | | 57.154 | 1.00 25.18 | |
| ATOM | 2048 | N | | | | 24.152 | 39.665 | | | AAAA |
| MOTA | 2049 | CA | ASP | | | 22.935 | 39.753 | 56.379 | 1.00 26.18 | AAAA |
| ATOM | 2050 | CB | ASP | Α | 258 | 22.950 | 38.830 | 55.149 | 1.00 25.52 | AAAA |
| ATOM | 2051 | CG | ASP | Α | 258 | 23.211 | 37.392 | 55.494 | 1.00 26.33 | AAAA |
| MOTA | 2052 | C | ASP | | | 21.649 | 39:574 | 57.178 | 1.00 26.74 | AAAA |
| | 2053. | ŏ | ASP | | | 20.571 | 39.823 | 56.643 | 1.00 26.57 | AAAA |
| ATOM | | | | | | | | | 1.00 26.85 | |
| MOTA | 2054 | | ASP | | | 23.014 | 37.029 | 56.675 | | AAAA |
| ATOM | 2055 | OD2 | ASP | A | 258 | 23.585 | 36.623 | 54.572 | 1.00 24.06 | AAAA |
| MOTA | 2056 | N | PRO | Α | 259 | 21.727 | 39.114 | 58.449 | 1.00 26.95 | AAAA |
| MOTA | 2057 | CD | PRO | Α | 259 - | 22.834 | 38.589 | 59.271 | 1.00 27.34 | AAAA |
| | 2058 | CA | PRO | | | 20.467 | 38.976 | 59.190 | 1.00 27.05 | AAAA |
| ATOM | - | | | | | | | 60.425 | 1.00 26.38 | AAAA |
| ATOM | 2059 | CB | PRO | | | 20.886 | 38.186 | | | |
| ATOM | 2060 | CG | PRO | | | 22.247 | 38.718 | 60.669 | 1.00 27.84 | AAAA |
| MOTA | 2061 | С | PRO | Α | 259 | 19.914 | 40.365 | 59.543 | 1.00 27.32 | AAAA |
| ATOM | 2062 | 0 | PRO | Α | 259 | 18.739 | 40.510 | 59.871- | 1.00 27.29 | AAAA |
| ATOM | 2063 | N | LEU | Δ | 260 | 20.771 | 41,383 | 59.452 | 1.00 26.97 | AAAA |
| | 2064 | CA | LEU | | | 20.389 | 42.763 | 59.752 | 1.00 26.74 | AAAA |
| ATOM | | | | | | | | | 1.00 27.21 | AAAA |
| ATOM | 2065 | CB | LEU | | | 21.621 | 43.680 | 59.680 | | |
| MOTA | 2066 | CG | LEU | | | 22.732 | 43.465 | 60.709 | 1.00 27.01 | AAAA |
| ATOM | 2067 | CD1 | LEU | Α | 260 | 23.889 | 44.380 | 60.408 | 1.00 25.51 | AAAA |
| ATOM | 2068 | CD2 | LEU | A | 260 . | 22.189 | 43.718 | 62.112 | 1.00 27.39 | AAAA |
| MOTA | 2069 | С | LEU | А | 260 | 19.295 | 43.351 | 58.865 | 1.00 26.47 | AAAA |
| | 2070 | ō | LEU | | | 19.278 | 43.137 | 57.649 | 1.00 26.72 | AAAA |
| ATOM | | | | | | | 44.126 | 59.494 | 1.00 26.32 | AAAA |
| MOTA | 2071 | N | LEU | | | 18.413 | | | | |
| MOTA | 2072 | CA | | | 261 | 17.283 | 44.808 | | 1.00 27.20 | AAAA |
| MOTA | 2073 | CB | LEU | A | 261 | 16.732 | 45.885 | 59.780 | 1.00 28.71 | AAAA |
| MOTA | 2074 | CG | LEU | Α | 261 | 15.644 | 46.789 | 59.190 | 1.00 29.24 | AAAA |
| ATOM | 2075 | CD1 | LEU | Α | 261 | 14.433 | 45.954 | 58.883 | 1.00 29.44 | AAAA |
| ATOM - | 2076 | | LEU | | | 15.284 | 47.906 | 60.162 | 1.00 29.72 | AAAA |
| | 2077 | c | LEU | | | 17.506 | 45.454 | 57.473 | 1.00 27.90 | AAAA |
| MOTA | | | | | | | | 56.577 | 1.00 28.21 | AAAA |
| ATOM | 2078 | 0 | | | 261 | 16.675 | 45.294 | | | |
| MOTA | 2079 | N | | | 262 | 18.597 | 46.202 | 57.310 | 1.00 27.61 | AAAA |
| ATOM | 2080 | CA | GLU | Α | 262 · | 18.887 | 46.877 | 56.043 | 1.00 26.92 | AAAA |
| ATOM | 2081 | CB | GLU | A | 262. | 19.949 | 47.955 | 56.241 | 1.00 25.85 | AAAA |
| MOTA | 2082 | CG | GLÜ | Α | 262 | 19.549 | 49.119 | 57.117 | 1.00 25.36 | AAAA |
| ATOM | 2083 | CD | | | 262 | 19.552 | 48.787 | 58.580 | 1.00 25.78 | AAAA |
| | | | GLU | | | 19.859 | 47.631 | 58.938 | 1.00 24.64 | AAAA |
| ATOM | 2084 | | | | | | | | 1.00 25.82 | AAAA |
| MOTA | 2085 | | GLU | | | 19.255 | 49.694 | 59.381 | | |
| MOTA | 2086 | С | GLU | Α | 262 | 19.346 | 45.995 | 54.882 | 1.00 28.79 | AAAA |
| MOTA | 2087 | 0 | GLU | A | 262 | 19.354 | 46.439 | 53.724 | 1.00 28.70 | AAAA |
| MOTA | 2088 | N | ASP | A | 263 | 19.743 | 44.758 | 55.179 | 1.00 29.57 | AAAA |
| ATOM | 2089 | CA | ASP | Α | 263 | 20.230 | 43.853 | 54.145 | 1.00 28.99 | AAAA |
| ATOM | 2090 | CB | | | 263 | 21.160 | 42.802 | 54.760 | 1.00 27.89 | AAAA |
| | 2091 | CG | | | 263 | 21.986 | 42.062 | 53.714 | 1.00 29.02 | · AAAA |
| ATOM | | | | | | | | 53.957 | 1.00 28.06 | AAAA |
| MOTA | 2092 | | ASP | | | 23.194 | 41.863 | | | |
| MOTA | 2093 | | ASP | | | 21.438 | 41.663 | 52.660 | 1.00 28.80 | AAAA |
| MOTA | 2094 | С | ASP | A | 263 | 19.066 | 43.197 | 53.431 | 1.00 29.73 | . AAAA |
| MOTA | 2095 | 0 | ASP | Α | 263 | 18.258 | 42.510 | 54.043 | 1.00 29.15 | AAAA |
| ATOM | 2096 | N | TYR | A | 264 | 19.002 | 43.416 | 52.122 | 1.00 31.25 | AAAA |
| | 2097 | CA | TYR | | | 17 925 | 42.888 | 51.306 | 1.00 32.43 | AAAA |
| ATOM | | | | | | | 43.558 | 49.938 | 1.00 34.53 | AAAA |
| ATOM | 2098 | CB | TYR | | | 17.913 | | | | |
| MOTA | 2099 | CG | | | 264 | 17.627 | 45.038 | 49.997 | 1.00 38.21 | AAAA |
| ATOM | 2100 | CD1 | TYR | Α | 264 | 18.664 | | 49.983 | 1.00 39.87 | AAAA |
| ATOM | 2101 | CE1 | TYR | A | 264 | 18.409 | 47.335 | 50.068 | 1.00 41.74 | AAAA |
| ATOM | 2102 | | TYR | | | 16.316 | 45.511 | 50.103 | 1.00 40.10 | AAAA |
| | 2103 | | TYR | | | 16.044 | 46.877 | 50.191 | 1.00 41.50 | AAAA |
| MOTA | | | | | | | 47.786 | 50.170 | 1.00 42.75 | AAAA |
| MOTA | 2104 | CZ | | | 264 | 17.095 | | | | |
| MOTA | 2105 | OH | | | 264 | 16.838 | 49.147 | 50.231 | 1.00 44.65 | AAAA |
| ATOM | 2106 | С | TYR | A | 264 | 17.897 | 41.385 | 51.135 | 1.00 32.50 | AAAA |
| ATOM | 2107 | 0 | TYR | A | 264 | 16.819 | 40.816 | 50.968 | 1.00 32.49 | AAAA |
| ATOM | 2108 | N | | | 265 | 19.064 | 40.740 | 51.171 | 1.00 32.64 | AAAA |
| | 2109 | CA | | | 265 | 19.122 | 39.281 | 51.036 | 1.00 31.92 | AAAA |
| ATOM | | | | | | | 38.823 | 50.617 | 1.00 32.75 | AAAA |
| MOTA | 2110 | CB | | | 265 | 20.525 | | | | |
| ATOM | 2111 | CG | | | 265 | 20.808 | 39.010 | 49.127 | 1.00 32.95 | AAAA |
| ATOM | 2112 | CD1 | LEU | A | 265 | 22.213 | 38.588 | 48.771 | 1.00 31.59 | AAAA |

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Figure 19-33

| ATOM | 2113 | CD2 | LEU | 7 265 | 10 003 | 20 166 | 40 363 | | |
|--------|------|-----|-------|--------|--------|--------|--------|------------|--------|
| | | | | | 19.803 | 38.166 | 48.361 | 1.00 34.62 | AAAA |
| MOTA | 2114 | С | | A 265 | 18.693 | 38.540 | 52.296 | 1.00 30.33 | AAAA |
| ATOM | 2115 | 0 | LEU . | A 265 | 19.024 | 37.375 | 52.484 | 1.00 30.30 | AAAA |
| MOTA | 2116 | N | SER . | A 266 | 17.945 | 39.230 | 53.147 | 1.00 29.23 | AAAA |
| ATOM | 2117 | CA | SER | A 266 | 17.434 | 38.649 | 54.371 | 1.00 29.72 | AAAA |
| ATOM - | 2118 | CB | | A 266 | 18.398 | 38.894 | 55.519 | 1.00 32.09 | |
| ATOM | 2119 | OG | | A 266 | 17.728 | | | | AAAA |
| | | | | | _ | 38.810 | 56.771 | 1.00 33.43 | AAAA |
| MOTA | 2120 | C | | A 266 | 16.115 | 39.290 | 54.698 | 1.00 28.71 | ÀAAA |
| MOTA | 2121 | 0 | SER . | A 266 | 15.924 | 40.473 | 54.444 | 1.00 29.67 | AAAA |
| ATOM | 2122 | N | LYS . | A 267 | 15.209 | 38.517 | 55.276 | 1.00 27.82 | AAAA |
| ATOM | 2123 | CA | LYS | A 267 | 13.908 | 39.045 | 55.654 | 1.00 27.56 | AAAA |
| MOTA | 2124 | CB | | A .267 | 12.821 | 38.076 | 55.222 | 1.00 28.75 | |
| ATOM | 2125 | CG | | A 267 | | | | | AAAA |
| | | | | | 12.733 | 37.922 | 53.718 | | AAAA |
| MOTA | 2126 | CD | | A 267 | | 39.223 | 53.053 | 1.00 30.13 | AAAA |
| ATOM | 2127 | CE | | A 267 | 12.303 | 39.036 | 51.546 | 1.00 31.86 | AAAA |
| MOTA | 2128 | NZ | LYS 2 | A 267 | 11.796 | 40.252 | 50.843 | 1.00 33.92 | -AAAA |
| ATOM | 2129 | С | LYS | A 267 | 13.800 | 39.327 | 57.152 | 1.00 27.18 | AAAA |
| ATOM | 2130 | 0 | LYS | A 267 | 12.707 | 39.591 | 57.665 | 1.00 27.18 | AAAA |
| ATOM | 2131 | N | | A 268 | 14.944 | 39.267 | 57.836 | 1.00 26.12 | |
| ATOM | 2132 | CA | | A 268 | | | | | AAAA |
| | | | | | 15.048 | 39.532 | 59.271 | 1.00 25.72 | AAAA |
| MOTA | 2133 | CB | | A 268 | 16.272 | 38.830 | 59.856 | 1.00 24.94 | AAAA |
| MOTA | 2134 | CG | | A 268 | 16.167 | 37.334 | 59.896 | 1.00 25.07 | AAAA |
| MOTA | 2135 | | PHE A | A 268 | 17.271 | 36.565 | 60.267 | 1.00.24.56 | AAAA |
| ATOM | 2136 | CD2 | PHE A | A 268 | 14.955 | 36.687 | 59.629 | 1.00 23.76 | AAAA |
| MOTA | 2137 | CE1 | PHE A | A 268 | 17.174 | 35.169 | 60.384 | 1.00 23.71 | AAAA |
| ATOM | 2138 | CE2 | PHE A | A 268 | 14.850 | 35.303 | 59.739 | 1.00 23.86 | AAAA |
| ATOM | 2139 | CZ | | A 268 | 15.966 | 34.542 | 60.121 | 1.00 23.68 | |
| ATOM | 2140 | c | | A 268 | | | | | AAAA |
| | | | | | 15.190 | 41.030 | 59.513 | 1.00 25.77 | AAAA |
| MOTA | 2141 | 0 | | A 268 | 15.811 | 41.734 | 58.726 | 1.00 25.81 | AAAA |
| MOTA | 2142 | N | | A 269 | | 41.524 | 60.595 | 1.00 26.02 | AAAA |
| MOTA | 2143 | CA | | A 269 | 14.718 | 42.943 | 60.890 | 1.00 26.58 | AAAA |
| MOTA | 2144 | CB | ASN A | A 269 | 13.330 | 43.584 | 61.058 | 1.00 25.47 | AAAA |
| ATOM | 2145 | CG | ASN A | A 269 | 12.379 | 43.252 | 59.906 | 1.00 25.37 | AAAA |
| MOTA | 2146 | OD1 | ASN A | | 12.761 | 43.260 | 58.734 | 1.00 23.82 | AAAA |
| ATOM | 2147 | | ASN A | | 11.123 | 42.985 | 60.245 | 1.00 24.03 | AAAA |
| ATOM | 2148 | C | | 269 | 15.540 | 43.112 | 62.169 | • | |
| | | ō | | | | | | 1.00 26.82 | AAAA |
| MOTA | 2149 | | | 269 | 15.089 | 43.715 | 63.150 | 1.00 27.98 | AAAA |
| ATOM | 2150 | N | | 270 | 16.744 | 42.559 | 62.149 | 1.00 26.07 | AAAA |
| MOTA | 2151 | CA | | 270 | 17.639 | 42.642 | 63.289 | 1.00 25.97 | AAAA |
| ATOM | 2152 | CB | | 1 270 | 18.634 | 41.479 | 63.265 | 1.00 23.76 | AAAA |
| MOTA | 2153 | CG | LEU A | 270 | 18.048 | 40.070 | 63.225 | 1.00 23.36 | AAAA |
| ATOM | 2154 | CD1 | LEU A | 270 | 19.115 | 39.090 | 63.710 | 1.00 21.90 | AAAA |
| ATOM | 2155 | CD2 | LEU A | 270 | 16.824 | 39.971 | 64.122 | 1.00 22.05 | AAAA |
| ATOM | 2156 | С | LEU A | | 18.420 | 43.961 | 63.360 | 1.00 27.13 | AAAA |
| ATOM | 2157 | Õ. | LEU A | | 18.475 | 44.750 | 62.399 | 1.00 25.99 | |
| | 2158 | | SER A | | | | | | AAAA |
| ATOM | | И | _ | | 19.038 | 44.176 | 64.517 | 1.00 27.97 | AAAA |
| ATOM | 2159 | CA | SER A | | 19.832 | 45.370 | 64.767 | 1.00 27.95 | AAAA |
| ATOM | 2160 | CB | SER A | | 19.235 | 46.137 | 65.943 | 1.00 27.32 | AAAA |
| ATCM | 2161 | OG | SER A | 271 | 19.184 | 45.297 | 67.089 | 1.00 27.90 | AAAA |
| MOTA | 2162 | С | SER A | 271 | 21.276 | 44.987 | 65.084 | 1.00 28.15 | AAAA |
| ATOM | 2163 | 0 | SER A | 271 | 21.574 | 43.832 | 65.401 | 1.00 26.99 | AAAA |
| ATOM | 2164 | N | ASN A | | 22.156 | 45.980 | | 1.00 28.96 | AAAA |
| ATOM | 2165 | CA | ASN A | | 23.590 | | | | |
| | 2166 | | | | | 45.861 | 65.266 | 1.00 29.54 | AAAA |
| ATOM | | CB | ASN A | | 24.247 | 47.243 | 65.223 | 1.00 30.96 | AAAA |
| MOTA | 2167 | CG | ASN A | | 24.647 | 47.640 | 63.850 | 1.00 31.20 | AAAA |
| ATOM | 2168 | | asn a | | 24.960 | 48.794 | 63.594 | 1.00 31.73 | AAAA |
| ATOM | 2169 | ND2 | ASN A | 272 | 24.670 | 46.674 | 62.948 | 1.00 31.93 | AAAA |
| MOTA | 2170 | С | ASN A | 272 | 23.821 | 45.309 | 66.645 | 1.00.29.63 | AAAA |
| ATOM | 2171 | 0 | ASN A | | 24.574 | 44.361 | 66.843 | 1.00 29.85 | AAAA |
| MOTA | 2172 | N | VAL A | | 23.180 | 45.959 | 67.600 | 1.00 29.77 | AAAA |
| | 2173 | | | | | | | | |
| MOTA | | | VAL A | | 23.290 | 45.602 | 68.994 | 1.00 30.89 | AAAA |
| ATOM | 2174 | CB | VAL A | | 22.436 | 46.576 | 69.816 | 1.00 31.61 | AAAA |
| MOTA | 2175 | | VAL A | | 22.716 | 46.403 | 71.293 | 1.00 33.17 | AAAA |
| MOTA | 2176 | | VAL A | | 22.740 | 47.998 | 69.372 | 1.00 31.82 | AAAA |
| ATOM | 2177 | C | VAL A | 273 | 22.883 | 44.144 | 69.266 | 1.00 30.74 | AAAA |
| MOTA | 2178 | 0 | VAL A | 273 | 23.550 | 43.431 | 70.022 | 1.00 31.23 | AAAA . |
| | | | | | _ | | • | | |

| | | | | | 224 | 21 705 | 43.7 | 06 | 68.659 | 1.00 | 30.25 | AAAA |
|--------|------|-----|------|-----|-------------|--------|-------|-------|---------|------|-----------|--------|
| ATOM | 2179 | N | ALA | A | 214 | 21.785 | 42.3 | | 68.840 | | 29.87 | AAAA |
| MOTA | 2180 | CA | ALA | | | 21.327 | 42.1 | | 68.112 | | 29.64 | AAAA |
| MOTA | 2181 | CB | ALA | | | 20.005 | | | 68.247 | | 29.35 | AAAA |
| ATOM | 2182 | c | ALA | | | 22.395 | 41.4 | | 68.778 | | 29.18 | AAAA |
| MOTA | 2183 | 0 | ALA | | | 22.707 | 40.3 | | 67.127 | | 29.30 | AAAA |
| MOTA | 2184 | N | PHE | | | 22.946 | 41.8 | _ | | | 28.91 | AAAA |
| ATOM | 2185 | CA | PHE | | | 23.991 | 41.1 | | 66.428 | | 28.77 | AAAA |
| MOTA | 2186 | CB | PHE | | | 24.375 | 41.9 | | 65.150 | | 28.08 | AAAA |
| MOTA | 2187 | CG | PHE | | | 25.354 | 41.1 | | 64.308 | | 28.92 | AAAA |
| MOTA | 2188 | | PHE | | | 25.015 | 39.9 | | 63.740 | | | AAAA |
| MOTA | 2189 | | PHE | | | 26.621 | 41.6 | | 64.077 | | 29:48 | AAAA |
| MOTA | 2190 | CE1 | PHE | | | 25.928 | 39.2 | | 62.945 | | 29.20 | AAAA · |
| ATOM | 2191 | CE2 | PHE | | | 27.546 | 40.9 | | 63.279 | | 29.24 | AAAA |
| ATOM - | 2192 | CZ | PHE | | | 27.193 | 39.7 | | 62.716 | | 28.30 | |
| MOTA | 2193 | С | PHE | | | 25.196 | 41.0 | | 67.351 | | 27.64 | AAAA |
| ATOM | 2194 | 0 | PHE | A | 275 | 25.728 | 39.9 | | 67.558 | | 28.65 | AAAA |
| MOTA | 2195 | И | LEU | A | 276 | 25.606 | 42. | | 67.902 | | 26.81 | AAAA |
| MOTA | 2196 | CA | LEU | Α | 276 | 26.732 | 42. | | 68.831 | | 27.38 | AAAA |
| MOTA | 2197 | CB | LEU | Α | 276 | 26.878 | 43. | | 69.353 | | 27.53 | AAAA |
| ATOM | 2198 | CG | LEU | | | 28.202 | 44. | | 69.928 | | 26.37 | AAAA |
| ATOM | 2199 | CD1 | LEU | Α | 276 | 27.923 | 45. | | 70.721 | | 25.71 | AAAA |
| ATOM | 2200 | CD2 | LEU | Α | 276 | 28.842 | | | 70.827 | | 27.06 | AAAA |
| ATOM | 2201 | С | LEU | Α | 276 | 26.486 | | | 70.021 | | 26.49 | AAAA |
| ATOM | 2202 | 0 | LEU | Α | 276 | 27.387 | | | 70.471 | | 25.26 | AAAA |
| ATOM | 2203 | N | LYS | Α | 277 | 25.257 | 41. | 322 | 70.524 | | 27.46 | AAAA |
| MOTA | 2204 | CA | LYS | Α | 277 | 24.894 | | | 71.642 | | 28.63 | AAAA |
| MOTA | 2205 | CB | LYS | Α | 277 | 23.542 | 40. | 862 | 72.223 | | 30.63 | AAAA |
| ATOM | 2206 | CG | LYS | Α | 277 | 23.590 | 42. | 029 | 73.153 | | 33.14 | AAAA |
| ATOM | 2207 | CD | LYS | Α | 277 | 22.599 | 41. | 791 | 74.268 | | 34.94 | AAAA |
| ATOM | 2208 | CE | LYS | A | 2 77 | 22.964 | 40. | 519 | 75.029 | | 36.17 | AAAA |
| ATOM | 2209 | NZ | LYS | A | 277 | 21.979 | 40. | 194 | 76.104 | | 38.64 | AAAA |
| ATOM | 2210 | C | LYS | Α | 277 | 24.846 | 38. | 997 | 71.297 | | 28.53 | AAAA |
| MOTA | 2211 | ō | | | 277 | 25.118 | 38. | 152 | 72.146 | | 28.45 | AAAA |
| ATOM | 2212 | N | | | 278 | 24.466 | 38. | 681 | 70.064 | | 28.47 | AAAA |
| MOTA | 2213 | CA | | | 278 | 24.404 | 37. | 280 | 69.656 | | 27.66 | AAAA |
| ATOM | 2214 | CB | | | 278 | 23.941 | . 37. | 181 | 68.201 | | 26.40 | AAAA |
| ATOM | 2215 | c | | | 278 | 25.833 | 36. | 754 | 69.820 | | 26.63 | AAAA |
| MOTA | 2216 | ō | | | 278 | 26.081 | 35. | 644 | 70.317 | | 25.19 | AAAA |
| ATOM | 2217 | N | | | 279 | 26.764 | | 616 | 69.427 | | 26.50 | AAAA |
| MOTA | 2218 | CA | | | 279 | 28.183 | 37. | 345 | 69.481 | | 25.83 | AAAA |
| ATOM | 2219 | CB | | | 279 | 28.934 | | 521 | 68.869. | | 26.35 | AAAA |
| ATOM | 2220 | CG | | | 279 | 30.413 | 38. | 319 | 68.796 | | 27.92 | AAAA |
| ATOM | 2221 | | PHE | | | 30.949 | 37. | 256 | 68.072 | | 28.58 | AAAA |
| ATOM | 2222 | | PHE | | | 31.280 | 39. | 201 | 69.434 | | 28.33 | AAAA |
| MOTA | 2223 | CE1 | | | 279 | 32.33 | 37. | 078 | 67.983 | | 28.22 | AAAA |
| ATOM | 2224 | CE2 | | | 279 | 32.66 | 5 39. | .030 | 69.349 | | 28.11 | AAAA |
| MOTA | 2225 | cz | | | 279 | 33.18 | 37. | 968 | 68.622 | | 28.21 | AAAA |
| | 2226 | c | | | 279 | 28.66 | 37. | .118 | 70.901 | 1.00 | 25.47 | AAAA |
| MOTA | 2227 | ŏ | | | 279 | 29.28 | | .091 | 71.202 | | 0 24.32 | AAAA |
| MOTA | 2228 | N | | | 280 | 28.38 | | 075 | 71.778 | | 0 25.12 | AAAA |
| ATOM | 2229 | CA | | | 280 | 28.84 | | 944 | 73.147 | 1.00 | 0 25.05 | AAAA |
| MOTA | 2230 | CB | | | 280 | 28.70 | 3 39. | .269 | 73.887 | 1.0 | 0 24.42 | AAAA |
| ATOM | 2231 | CG | | | 280 | 29.68 | | 300 | 73.364 | 1.0 | 0 24.56 | AAAA |
| ATOM | 2232 | | ASN | | | 30.84 | | 980 | 73.080 | 1.0 | 0 23.24 | AAAA |
| MOTA | 2233 | | ASN | | | 29.23 | | .543 | 73.249 | | 0 24.59 | AAAA |
| ATOM | 2234 | C | | | 280 | 28.21 | | 814 | 73.925 | 1.0 | 0 24.79 | AAAA |
| ATCM | | ō | | | 280 | 28.82 | | .272 | 74.825 | 1.0 | 0 24.96 | AAAA |
| MOTA | 2235 | Ŋ | | | 281 | 26.99 | | 444 | 73.565 | 1.0 | 0 24.87 | AAAA |
| MOTA | 2236 | CA | TIF | 3 | 281 | 26.33 | | .337 | 74.220 | 1.0 | 0 24.80 | AAAA |
| ATOM | 2237 | | 71.2 | 3 | 281 | 24.86 | | . 252 | 73.780 | 1.0 | 0 24.40 | AAAA |
| MOTA | 2238 | CB | ILE | | 281 | 24.29 | · | .907 | 74.124 | 1.0 | 0 25.03 | AAAA |
| MOTA | 2239 | CG2 | ILE | | 281 | 24.07 | | .386 | 74.424 | | 0 24.70 | AAAA |
| ATOM. | 2240 | COT | ILE | , A | 281 | 22.61 | | .379 | 74.069 | | 0 26.49 | AAAA |
| ATOM | 2241 | | | | 281 | 27.04 | _ | .027 | 73.884 | 1.0 | 0 25.21 | AAAA |
| Mota | 2242 | . C | | | | 27.22 | | .170 | 74.750 | 1.0 | 0 24.97 | AAAA |
| MOTA | 2243 | , O | | | 281 | 27.22 | 0 33 | .866 | 72.620 | 1.0 | 0 25.98 | AAAA |
| ATCM | 2244 | И | VAL | | 282 | 21.44 | | | • | | · · · · · | • |
| | | | • | | | | | | | | | |

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| MOTA | 2245 | CA | VAL | A | 282 | | 28.150 | 32.656 | 72.193 | 1.00 25.19 | AAAA c |
|--------|------|-----|-----|---|-----|-----|--------|--------|--------|------------|--------|
| ATOM | 2246 | CB | | | 282 | | 28.451 | 32.666 | 70.677 | 1.00 23.83 | |
| ATOM | 2247 | | VAL | | - | | 29.315 | 31.470 | 70.311 | 1.00 23.58 | |
| | _ | | | | | | | 32.633 | 69.899 | | |
| MOTA | 2248 | | VAL | | | | 27.173 | | | 1.00 22.73 | |
| MOTA | 2249 | С | | | 282 | | 29.478 | 32.553 | 72.936 | 1.00 25.7 | |
| MOTA | 2250 | 0 | VAL | A | 282 | | 29.928 | 31.457 | 73.275 | 1.00 25.33 | L AAAA |
| MOTA | 2251 | N | ARG | Α | 283 | | 30.100 | 33.702 | 73.176 | 1.00 26.90 | AAAA (|
| ATOM | 2252 | CA | | | 283 | | 31.372 | 33.760 | 73.885 | 1.00 28.8 | |
| | | CB | | | 283 | | 32.027 | 35.131 | 73.684 | 1.00 28.1 | _ |
| MOTA | 2253 | | | | | | | | | | |
| ATOM | 2254 | CG | | | 283 | | 32.364 | 35.440 | 72.240 | 1.00 27.22 | |
| ATOM | 2255 | CD. | ARG | A | 283 | | 32.821 | 36.862 | 72.098 | 1.00 27.0 | B AAAA |
| ATOM | 2256 | ΝE | ARG | Α | 283 | | 34.035 | 37.116 | 72.854 | 1.00 26.73 | AAAA |
| MOTA | 2257 | CZ | ARG | Α | 283 | | 34.514 | 38.327 | 73.091 | 1.00 26.83 | AAAA S |
| MOTA | 2258 | | ARG | | | | 33.873 | 39.384 | 72.626 | 1.00 27.3 | |
| | 2259 | | ARG | | | | 35.622 | 38.484 | 73.798 | 1.00 26.9 | |
| MOTA | | | | | | | | | | | |
| MOTA | 2260 | C | | | 283 | | 31.183 | 33.494 | 75.376 | 1.00 30.7 | |
| ATOM | 2261 | 0 | | | 283 | | 32.086 | 32.981 | 76.027 | 1.00 30.6 | |
| MOTA | 2262 | N | GLU | A | 284 | • | 30.014 | 33.842 | 75.911 | 1.00 32.7 | aaaa 1 |
| ATOM | 2263 | CA | GLU | Α | 284 | | 29.735 | 33.623 | 77.323 | 1.00 35.5 | 3 AAAA |
| ATOM | 2264 | CB | GLU | Α | 284 | | 28.482 | 34.391 | 77.751 | 1.00 37.3 | |
| | 2265 | CG | | | 284 | | 28.538 | 35.854 | 77.392 | 1.00 41.7 | |
| MOTA | | | | | | | | | 77.754 | | |
| ATOM | 2266 | CD | | | 284 | | 27.272 | 36.631 | | 1.00 45.2 | |
| MOTA | 2267 | | GLU | | | | 26.151 | 36.078 | 77.610 | 1.00 46.6 | |
| ATOM | 2268 | OE2 | GLU | Α | 284 | | 27.405 | 37.817 | 78.148 | 1.00 46.9 | 4 AAAA |
| MOTA | 2269 | С | GLU | Α | 284 | | 29.524 | 32.133 | 77.564 | 1.00 36.2 | 5 AAAA |
| MOTA | 2270 | 0 | GLU | Α | 284 | | 29.920 | 31.593 | 78.601 | 1.00 37.8 | 5 AAAA |
| ATOM | 2271 | N | | | 285 | | 28.916 | 31.464 | 76.591 | 1.00 35.2 | |
| | 2272 | CA | | | 285 | | 28.637 | 30.041 | 76.708 | 1.00 33.8 | |
| MOTA | | | | | 285 | , . | | 29.619 | 75.737 | 1.00 33.7 | |
| ATOM | 2273 | CB. | | | | | 27.505 | | | | |
| MOTA | 2274 | | VAL | | | | 27.201 | 28.137 | 75.888 | 1.00 32.5 | |
| ATOM | 2275 | CG2 | VAL | A | 285 | | 26.254 | 30.457 | 76.001 | 1.00 32.7 | |
| ATOM | 2276 | С | VAL | Α | 285 | | 29.847 | 29.149 | 76.456 | 1.00 33.4 | 7 AAAA |
| ATOM | 2277 | 0 | VAL | A | 285 | | 30.140 | 28.262 | 77.257 | 1.00 34.2 | AAAA 8 |
| ATOM | 2278 | N | | | 286 | | 30.568 | 29.389 | 75.364 | 1.00 32.3 | |
| | 2279 | CA | | | 286 | | 31.706 | 28.535 | 75.036 | 1.00 29.9 | |
| ATOM | | | | | 286 | | 31.533 | 27.960 | 73.635 | 1.00 29.7 | |
| MOTA | 2280 | CB | | | | | | | | | |
| MOTA | 2281 | CG | | | 286 | | 30.267 | 27.179 | 73.444 | 1.00 28.6 | |
| atom | 2282 | | PHE | | | | 29.152 | 27.772 | 72.863 | 1.00 28.7 | |
| ATOM | 2283 | CD2 | PHE | Α | 286 | | 30.197 | 25.837 | 73.827 | 1.00 28.5 | 5 AAAA |
| MOTA | 2284 | CE1 | PHE | A | 286 | | 27.983 | 27.039 | 72.660 | 1.00 29.0 | 4 AAAA |
| ATOM | 2285 | CE2 | PHE | A | 286 | | 29.037 | 25.095 | 73.629 | 1.00 28.1 | AAAA e |
| ATOM | 2286 | CZ | | | 286 | | 27.929 | 25.694 | 73.045 | 1.00 28.7 | |
| | 2287 | Č | | | 286 | | 33.106 | 29.113 | 75.132 | 1.00 29.1 | |
| MOTA | | | | | | | | 28.436 | 74.760 | 1.00 28.5 | |
| ATOM. | 2288 | 0 | | | 286 | | 34.073 | | | | |
| MOTA | 2289 | N | | | 287 | | 33.224 | 30.341 | 75.637 | 1.00 28.4 | |
| ATOM | 2290 | CA | | | 287 | | 34.525 | 30.987 | 75.744 | 1.00 27.0 | |
| ATOM | 2291 | С | GLY | Α | 287 | | 34.932 | 31.611 | 74.419 | 1.00 26.6 | |
| MOTA | 2292 | 0 | GLY | A | 287 | | 34.088 | 32.042 | 73.649 | 1.00 27.1 | 3 AAAA |
| ATOM | 2293 | N | GLU | Α | 288 | | 36.227 | 31.665 | 74.146 | 1.00 27.2 | AAAA 0 |
| | 2294 | CA | | | 288 | | 36.719 | 32.238 | 72.900 | 1.00 27.5 | |
| ATOM | | CB | GLU | | | | 38.073 | 32.923 | 73.108 | 1.00 28.1 | |
| Mota | 2295 | | | | | | | | | | |
| MOTA | 2296 | CG | GLU | | | | 38.036 | 34.177 | 73.959 | 1.00 28.8 | |
| ATOM . | 2297 | CD | GLU | | | | 37.329 | 35.330 | 73.279 | 1.00 29.5 | |
| MOTA | 2298 | OE1 | GLU | Α | 288 | | 37.807 | 35.813 | 72.243 | 1.00 29.9 | 4 AAAA |
| ATOM | 2299 | OE2 | GLU | A | 288 | | 36.281 | 35.761 | 73.782 | 1.00 31.8 | 9 AAAA |
| ATOM | 2300 | С | GLU | | | | 36.877 | 31.158 | 71.843 | 1.00 27.4 | |
| | | ŏ | | | 288 | | 37.169 | 30.007 | 72.162 | 1.00 27.8 | |
| ATOM | 2301 | | | | | | | | 70.589 | 1.00 26.5 | |
| MOTA | 2302 | N | GLY | | | | 36.663 | 31.547 | | | |
| ATOM | 2303 | CA | GLY | | | | 36.795 | 30.638 | 69.466 | 1.00 25.2 | |
| MOTA | 2304 | С | GLY | A | 289 | | 37.285 | 31.414 | 68.254 | 1.00 24.5 | |
| ATOM | 2305 | 0 | GLY | | | | 37.635 | 32.586 | 68.369 | 1.00 24.4 | AAAA 0 |
| MOTA | 2306 | N | VAL | | | | 37.320 | 30.765 | 67.095 | 1.00 24.0 | 4 AAAA |
| | 2307 | CA | VAL | | | | 37.756 | 31.407 | 65.863 | 1.00 23.7 | |
| ATOM | | | | | | | | • | 64.867 | 1.00 24.9 | - |
| ATOM | 2308 | CB | VAL | | | | 38.288 | 30.346 | | | |
| MOTA | 2309 | | VAL | | | | 38.835 | 31.012 | 63.596 | 1.00 22.7 | |
| MOTA | 2310 | CG2 | VAL | A | 290 | | 39.375 | 29.506 | 65.555 | 1.00 24.7 | 4 AAAA |

| | | | | | | | | _ | | |
|--------|------|--------------|-------|-------|---|------------------|------------------|------------------|--------------------------|--------------|
| ATOM . | 2311 | С | VAL A | 290 | | 36.536 | 32.122 | 65.277 | 1.00 23.90 | AAAA |
| ATOM | 2312 | | VAL A | | | 35.497 | 31.502 | 65.100 | 1.00 25.15 | AAAA |
| ATOM | 2313 | N | TYR A | 291 | | 36.662 | 33.415 | 64.976 | 1.00 23.09 | AAAA |
| ATOM | 2314 | CA | TYR A | 291 | | 35.544 | 34.211 | 64.446 | 1.00 21.41 | AAAA |
| MOTA | 2315 | CB | TYR A | 291 | | 35.472 | 35.540 | 65.193 | 1.00 20.57 | AAAA |
| ATOM | 2316 | CG | TYR A | | | 35.511 | 35:346 | 66.677 | 1.00 19.87 | AAAA |
| ATOM | 2317 | CD1 | TYR A | 291 | | 36.596 | 35.782 | 67.432 | 1.00 20.86 | AAAA |
| MOTA | 2318 | CEl | TYR A | 291 | • | 36.677 | 35.513 | 68.793 | 1.00 21.47 | AAAA |
| ATOM | 2319 | CD2 | TYR A | 291 | | 34.509 | 34:647 | 67.318 | 1.00 20.90 | AAAA |
| MOTA | 2320 | CE2 | TYR A | 291 | | 34.579 | 34.372 | 68.675 | 1.00 21.90 | AAAA |
| ATOM | 2321 | CZ | TYR A | 291 | | 35.661 | 34.800 | 69.403 | 1.00 21.25 | AAAA |
| MOTA | 2322 | OH | TYR A | 291 | | 35.737 | 34.469 | 70.730 | 1.00 23.75 | AAAA |
| ATOM | 2323 | C | TYR A | 291 | | 35.607 | 34.483 | 62.946 | 1.00 21.25 | AAAA |
| MOTA | 2324 | 0 | TYR A | 291 | | 36.573 | 35.077 | 62.451 | 1.00 21.10 | AAAA |
| ATOM | 2325 | N | LEU A | 292 | | 34.557 | 34.084 | 62.231 | 1.00 20.92 | AAAA |
| ATOM | 2326 | CA | LEU A | 292 | | 34.518 | 34.260 | 60.779- | 1.00 20.92 | AAAA |
| ATOM | 2327 | CB | LEU A | 292 | | 34.235 | 32.916 | 60.080 | 1.00 19.93 | AAAA |
| ATOM | 2328 | CG | LEU A | | | 35.104 | 31.688 | 60.399 | 1.00 17.31 | AAAA |
| MOTA | 2329 | CD1 | LEU A | A 292 | | 34.685 | 30.515 | 59.528 | 1.00 16.05 | AAAA |
| ATOM | 2330 | CD2 | LEU A | A 292 | | 36.552 | 32.000 | 60.163 | 1.00 18.07 | AAAA |
| ATOM | 2331 | С | LEU A | A 292 | | 33.515 | 35.288 | 60.283 | 1.00 21.12 | AAAA |
| MOTA | 2332 | 0 | LEU A | A 292 | | 32.652 | 35.741 | 61.020 | 1.00 20.70 | AAAA |
| ATOM | 2333 | N | GLY F | A 293 | | 33.660 | 35.660 | 59.017 | 1.00 21.74 | AAAA |
| ATOM | 2334 | CA | GLY F | A 293 | | 32.752 | 36.612 | 58.410 | 1.00 21.48 | AAAA |
| ATOM | 2335 | С | GLY A | A 293 | | 31.612 | 35.856 | 57.770 | 1.00 21.65 | AAAA AAAA |
| ATOM | 2336 | 0 | GLY F | | | 31.237 | 34.790 | 58.235 | 1.00 22.25 | AAAA |
| ATOM | 2337 | N | | A 294 | | 31.060 | 36.392 | 56.691 | 1.00 22.66 | AAAA |
| MOTA | 2338 | CA | | A 294 | | 29.957 | 35.714 | 56.034 | 1.00 23.61 | AAAA |
| ATOM | 2339 | С | GĻX 1 | A 294 | | 29.180 | 36.653 | 55.146 | 1.00 24.56 | AAAA |
| ATOM - | 2340 | 0 | | A 294 | | 29.679 | 37.727 | 54.790 | 1.00 25.54 | AAAA |
| ATOM | 2341 | N | | A 295 | | 27.956 | 36.265 | 54.794 | 1.00 24.06 | AAAA |
| ATOM | 2342 | CA | | A 295 | | 27.139 | 37.093 | 53.927 | 1.00 22.78 1.00 23.11 | AAAA |
| ATOM | 2343 | С | | A 295 | | 26.902 | 38.479 | 54.483 | 1.00 23.11 | AAAA |
| ATOM | 2344 | Ο. | | A 295 | | 26.870 | 38.676 | 55.696 | 1.00 22.78 | AAAA |
| MOTA | 2345 | N | | A 296 | | 26.733 | 39.442 | 53.584 53.993 | 1.00 23.44 | AAAA |
| MOTA | 2346 | CA | | A 296 | • | 26.497 | 40.813 | 52.718 | 1.00 23.72 | AAAA |
| ATOM | 2347 | С | | A 296 | | 26.471 | 41.618 | 52.710 | 1.00 23.73 | AAAA |
| ATOM | 2348 | 0 | | A 296 | | 27.474 | 41.661 42.280 | 52.425 | 1.00 23.41 | AAAA |
| ATOM | 2349 | N | | A 297 | | 25.356 | 42.200 | 51.163 | 1.00 22.71 | AAAA |
| MOTA | 2350 | CA | | A 297 | | 25.282 | 42.294 | | 1.00 21.55 | AAAA |
| ATOM | 2351 | CB | | A 297 | | 24.252 24.496 | 40.809 | 50.317 | 1.00 21.93 | AAAA |
| MOTA | 2352 | CG | | A 297 | | 24.436 | 40.016 | 51.375 | 1.00 20.95 | AAAA |
| MOTA | 2353 | CDI | TYR . | A 291 | | 24.400 | 38.678 | 51.481 | 1.00 21.59 | AAAA |
| MOTA | 2354 | CEI | TYR | A 207 | | 25.320 | 40.217 | 49.358 | 1.00 21.71 | AAAA |
| atom | 2355 | CDZ | TYR . | A 207 | | 25.688 | 38.900 | 49.451 | 1.00 21.99 | AAAA |
| MOTA | 2356 | | TIL. | A 297 | | 25.242 | | 50.511 | 1.00 22.18 | AAAA |
| MOTA | 2357 | CZ | TIN. | A 297 | | 25.721 | | 50.615 | 1.00 21.35 | AAAA |
| ATOM | 2358 | OH | | A 297 | | 25.042 | | 51.225 | 1.00 22.90 | AAAA |
| MOTA | 2359 | C | | A 297 | | 25.106 | | 50.203 | 1.00 23.17 | AAAA |
| ATOM | 2360 | 0 | | A 298 | | 24.772 | | | 1.00 22.47 | AAAA |
| MOTA | 2361 | N | nio. | A 298 | | 24.572 | | | 1.00 24.27 | AAAA |
| MOTA | 2362 | CA | HIC | A 298 | | 23.468 | | | 1.00 23.17 | AAAA |
| MOTA | 2363 | CB | HIG. | A 298 | | 23.097 | _ | . 53.572 | | AAAA |
| ATOM | 2364 | CG | HIS | A 298 | | 23.588 | | | | AAAA |
| MOTA | 2365 | לבוט לחוז | HIS | A 298 | | 22.199 | | | 1.00 23.14 | AAAA |
| MOTA | 2366 | CEI | DTH | A 298 | | 22.151 | | | 1.00 23.31 | AAAA |
| ATOM | 2367 | がほう | HTS | A 298 | | 22.986 | | | 1.00 23.62 | AAAA |
| MOTA | 2368 | C | HTS | A 298 | | 25.886 | · · · · | | 1.00 25.17 | AAAA |
| MOTA | 2369 | o | HTS | A 298 | | 26.282 | | 54.239 | 1.00 24.47 | AAAA |
| MOTA | 2370 | N | DBU | A 299 | | 26.563 | | | 1.00 26.37 | AAAA |
| MOTA | 2371 | CD | | A 299 | | 26.178 | | | | AAAA |
| ATOM | 2372 | CA | PRO | A 299 | | 27.840 | | | 1.00 27.31 | AAAA |
| MOTA | 2373 | CB | | A 299 | | 28.156 | _ | 51.630 | | AAAA |
| MOTA | 2374 | CG | | A 299 | | 26.743 | | | 1.00 27.57 | AAAA |
| MOTA | 2375 | _ | | A 299 | | 27.824 | | | 1.00 27.77 | AAAA |
| MOTA | 2376 | - | | | | | | - | | • |
| | | | | | | | | | | |

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| ATOM | 2377 | 0 | PRO | Α | 299 | 28.755 | 48.826 | 54.939 | 1.00.3 | 28.04 | AAAA |
|--------|-------|------|-------|----|-------|--------|--------|----------|--------|-------|-------|
| ATOM | 2378 | N | | | 300 | 26.769 | 49.794 | 54.452 | 1.00 | | |
| | | | _ | | | | | | | | AAAA |
| ATOM | 2379 | CA | TYR | A | 300 | 26.629 | 50.477 | 55.740 | 1.00 | 27.59 | AAAA |
| ATOM | 2380 | CB | TYR | Α | 300 | 25.425 | 51.437 | 55.700 | 1.00 | 30.57 | AAAA |
| ATOM | 2381 | CG | | | 300 | 25.516 | 52.599 | 54.718 | 1.00 | | AAAA |
| | | | | | | | | | | | |
| ATOM - | 2382 | CD1 | | | 300 | 26.181 | 52.464 | 53.491 | 1.00 | | AAAA |
| MOTA | 2383 | CE1 | TYR | Α | 300 | 26.160 | 53.487 | 52.538 | 1.00 | 33.91 | AAAA |
| ATOM | 2384 | CD2 | TYR | Δ | 300 | 24.837 | 53.801 | 54.969 | 1.00 | 34 19 | AAAA |
| | | | | | | | | | | | |
| MOŢA | 2385 | CE2 | | | 300 | 24.809 | 54.830 | 54.018 | 1.00 | | AAAA |
| MOTA | 2386 | CZ | TYR | Α | 300 | 25.468 | 54.657 | 52.807 | 1.00 | 34.56 | AAAA |
| MOTA | 2387 | OH | TYR | Α | 300 | 25.389 | 55.630 | 51.844 | 1.00 | 36.05 | AAAA |
| | 2388 | C | | | 300 | 26.454 | 49.538 | 56.936 | | 26.48 | • |
| ATOM | | | | | - | | | - | | | AAAA |
| ATOM | 2389 | 0 | TYR | Α | 300 - | 27.073 | 49.726 | 57.979 - | 1.00 | 25.81 | AAAA |
| MOTA | 2390 | N | ALA | Α | 301 | 25.581 | 48.547 | 56.791 | 1.00 | 25.41 | AAAA |
| ATOM | 2391 | CA | AT.A | Δ | 301 | 25.328 | 47.606 | 57.865 | 1 00 | 24.64 | AAAA |
| | | | | | | | | | | | |
| MOTA | 2392` | CB | | | 301 | 24.164 | 46.731 | 57.511 | | 25.32 | -AAAA |
| ATOM | 2393 | С | ALA | A | 301 | 26.568 | 46.775 | 58.067 | 1.00 | 25.53 | AAAA |
| ATOM | 2394 | 0 | ALA | Α | 301 | 27.030 | 46.567 | 59.194 | 1.00 | 26.39 | AAAA |
| | 2395 | N | | | 302 | 27.108 | 46.304 | 56.950 | | 25.83 | AAAA |
| MOTA | | | | | | | | | | | |
| MOTA | 2396 | CA | LEU | A | 302 | 28.323 | 45.500 | 56.926 | 1.00 | 26.32 | AAAA |
| ATOM | 2397 | CB | LEU | A | 302 | 28.782 | 45.378 | 55.479 | 1.00 | 27.38 | AAAA |
| ATOM | 2398 | CG | | | 302 | 30.081 | 44.723 | 55.024 | 1.00 | 28.18 | AAAA |
| | | | | | | | | | | | |
| ATOM | 2399 | | LEU | | | 30.119 | 44.840 | 53.502 | | 29.32 | AAAA |
| ATOM | 2400 | CD2 | LEU | A | 302 | 31.296 | 45.389 | 55.613 | 1.00 | 27.38 | AAAA |
| MOTA | 2401 | С | LEU | Α | 302 | 29.398 | 46.187 | 57.764 | 1.00 | 26.41 | AAAA |
| ATOM | 2402 | 0 | | | 302 | 29.874 | 45.648 | 58.755 | | 26.62 | AAAA |
| | | | _ | | | | | | | | |
| MOTA | 2403 | N | | | 303 | 29.756 | 47.397 | 57.353 | | 26.50 | AAAA |
| ATOM | 2404 | CA | ALA | Α | 303 | 30.778 | 48.176 | 58.022 | 1.00 | 25.92 | AAAA |
| MOTA | 2405 | CB | ALA | Α | 303 | 31.001 | 49.475 | 57.277 | 1.00 | 25.24 | AAAA |
| MOTA | 2406 | C | | | 303 | 30.490 | 48.464 | 59.487 | | 26.03 | AAAA |
| | | | | | | | | | | | |
| MOTA | 2407 | 0 | | | 303 | 31.325 | 48.175 | 60.340 | | 26.95 | AAAA |
| MOTA | 2408 | N | ARG | Α | 304 | 29.322 | 49.028 | 59.792 | 1.00 | 25.29 | AAAA |
| MOTA | 2409 | CA | ARG | Α | 304 | 28.999 | 49.353 | 61.179 | 1.00 | 23.46 | AAAA |
| MOTA | 2410 | CB | ARG | Δ | 304 . | 27.641 | 50.059 | 61.291 | 1.00 | 23.78 | AAAA |
| | | | | | 304 | 27.553 | | 60.629 | | 24.59 | AAAA |
| MOTA | 2411 | -CG | | | | | 51.451 | | | | |
| ATOM | 2412 | CD | | | 304 | 26.302 | 52.223 | 61.091 | | 25.85 | AAAA |
| MOTA | 2413 | NE | ARG | Α | 304 | 25.067 | 51.465 | 60.869 | 1.00 | 27.54 | AAAA |
| ATOM | 2414 | CZ | ARG | Α | 304 | 23.978 | 51.547 | 61.637 | 1.00 | 28.36 | AAAA |
| ATOM | 2415 | | ARG | | | 23.957 | 52.362 | 62.695 | | 26.48 | AAAA |
| | | | | | | | | | | | |
| MOTA | 2416 | | ARG | | | 22.910 | 50.794 | 61.358 | | 28.45 | AAAA |
| ATOM | 2417 | С | ARG | A | 304 | 28.991 | 48.118 | 62.053 | 1.00 | 23.18 | AAAA |
| ATOM | 2418 | 0 | ARG | Α | 304 | 29.591 | 48.099 | 63.135 | 1.00 | 22.26 | AAAA |
| ATOM | 2419 | N | | | 305 | 28.330 | 47.075 | 61.560 | 1 00 | 23.20 | AAAA |
| | | | | | | | | | | | |
| ATOM | 2420 | CA | | | 305 | 28.200 | 45.817 | 62.292 | | 22.33 | AAAA |
| MOTA | 2421 | CB | ALA | A. | 305 | 27.319 | 44.866 | 61.516 | 1.00 | 22.17 | AAAA |
| ATOM | 2422 | С | ALA | A | 305 | 29.516 | 45.137 | 62.621 | 1.00 | 22.27 | AAAA |
| ATOM | 2423 | 0 | A.T.A | А | 305 | 29.763 | 44.757 | 63.760 | 1.00 | 22.48 | AAAA |
| | | | | | 306 | | | 61.620 | | 22.57 | AAAA |
| MOTA | 2424 | N | | | | 30.366 | 44.969 | | | | |
| ATOM | 2425 | CA | TRP | А | 306 | 31.634 | 44.307 | 61.861 | | 21.28 | AAAA |
| ATOM | 2426 | CB | TRP | Α | 306 | 32.279 | 43.885 | 60.553 | 1.00 | 21.07 | AAAA |
| ATOM | 2427 | CG | TRP | Δ | 306 | 31.703 | 42.618 | 60.004 | 1.00 | 20.75 | AAAA |
| | | | | | | | | | | 19.54 | |
| MOTA | 2428 | CDZ | TRP | A | 300 | 31.886 | 42.103 | 58.683 | | | AAAA |
| MOTA | 2429 | | TRP | | | 31.352 | 40.795 | 58.668 | | 19.18 | AAAA |
| ATOM | 2430 | CE3 | TRP | A | 306 | 32.456 | 42.616 | 57.510 | 1.00 | 19.59 | AAAA |
| ATOM | 2431 | CDI | TRP | Δ | 306 | 31.071 | 41.632 | 60.713 | | 20.51 | AAAA |
| | | | | | | | | | | | |
| MOTA | 2432 | | TRP | | | 30.864 | 40.537 | 59.922 | | 19.74 | |
| MOTA | 2433 | | TRP | | | 31.368 | 39.990 | 57.524 | | 19.18 | AAAA |
| MOTA | 2434 | CZ3. | TRP | Α | 306 | 32.474 | 41.810 | 56.367 | 1.00 | 18.98 | AAAA |
| | 2435 | | TRP | | | 31.933 | 40.513 | 56.388 | | 19.21 | AAAA |
| MOTA | | | | | | | | | | 20.80 | |
| ATOM | 2436 | С | TRP | | | 32.571 | 45.159 | 62.674 | | | AAAA |
| MOTA | 2437 | o | TRP | | | 33.459 | 44.630 | 63.341 | | 20.55 | AAAA. |
| ATOM | 2438 | N | THR | | | 32.373 | 46.475 | 62.614 | 1.00 | 20.17 | AAAA |
| | | CA | THR | | | 33.175 | 47.399 | 63.407 | | 20.54 | AAAA |
| MOTA | 2439 | | | | | | | | | | |
| MOTA | 2440 | CB | THR | | | 32.861 | 48.881 | 63.045 | | 21.09 | AAAA |
| MOTA | 2441 | OG1 | THR | A | 307 | 33.329 | 49.159 | 61.718 | | 21.25 | AAAA |
| ÄTOM | 2442 | CGS | THR | А | 307 | 33.523 | 49.839 | 64.030 | 1.00 | 20.09 | AAAA |
| W1013 | | | | | | | 055 | - | | | |



| 3 (TO) (| 2443 | С | THR A 3 | 07 | 32.853 | 47.135 | 64.893 | 1.00 20.88 | AAAA |
|----------|-------|-----|---------|-----|--------|---------|----------|------------|--------|
| MOTA | | | | | 33.738 | 47.175 | 65.747 | 1.00 21.89 | AAAA |
| MOTA | 2444 | 0 | THR A 3 | | | | 65.192 | 1.00 20.10 | AAAA |
| ATOM | 2445 | N | LEU A 3 | | 31.588 | 46.851 | | | |
| MOTA | 2446 | CA | LEU A 3 | 808 | 31.189 | 46.543 | 66.559 | 1.00 21.10 | AAAA |
| ATOM | 2447 | CB | LEU A 3 | 808 | 29.671 | 46.340 | 66.644 | 1.00 20.99 | AAAA |
| | 2448 | CG | LEU A 3 | | 28.897 | 47.656 | 66.674 | 1.00 21.54 | AAAA |
| MOTA | | | | | 27.397 | 47.473 | 66.411 | 1.00 19.91 | AAAA |
| MOTA | 2449 | | LEU A 3 | | | | 68.045 | 1.00 21.04 | AAAA |
| MOTA | 2450 | CD2 | LEU A 3 | - | 29.177 | 48.283 | | | |
| MOTA | 2451 | С | LEU A 3 | 308 | 31.886 | 45.284 | 67.052 | 1.00 21.98 | AAAA |
| ATOM | 2452 | 0 | LEU A 3 | 808 | 32.284 | 45.186 | 68.215 | 1.00 22.17 | AAAA |
| | 2453 | Ŋ | ILE A | | 32.023 | 44.310 | 66.165 | 1.00 22:32 | AAAA |
| MOTA | | | | | 32.658 | 43.069 | 66.544 | 1.00 23.12 | AAAA |
| ATOM | 2454 | CA | ILE A | | | | 65.413 | 1.00 22.33 | AAAA . |
| MOTA | 2455 | CB | ILE A 3 | | 32.590 | 42.016 | | | AAAA |
| MOTA | 2456 | | ILE A | | 33.356 | 40.787 | 65.827 | 1.00 21.76 | |
| ATOM | 2457 | CG1 | ILE A | 309 | 31.140 | 41.678 | 65.061 | 1.00 22.16 | AAAA |
| | 2458 | | ILE A | | 30.366 | 41.037 | 66.166 | 1.00 22.01 | AAAA |
| MOTA | | | ILE A | | 34.115 | 43.377 | 66,790 | 1.00 24.52 | AAAA |
| MOTA | 2459 | C | | | | 42.828 | 67.709 | 1.00 25.72 | AAAA |
| ATOM | 2460 | 0 | ILE A | | 34.734 | | | 1.00 24.70 | AAAA |
| ATOM | 2461 | N | TRP A | 310 | 34.673 | 44.253 | 65.957 | | |
| MOTA | 2462 | CA | TRP A | 310 | 36.075 | 44.570 | 66.099 | 1.00 24.20 | AAAA |
| ATOM | 2463 | CB | TRP A | 310 | 36,587 | 45.417 | 64.944 | 1.00 23.29 | AAAA |
| | 2464 | CG | TRP A | | 38.040 | 45.712 | 65.123 | 1.00 23.17 | AAAA |
| MOTA | | | | | 39.104 | 44.752 | 65.257 | 1.00 21.36 | AAAA |
| MOTA | 2465 | CDZ | TRP A | 310 | | | 65.490 | 1.00 20.62 | AAAA |
| ATOM | 2466 | | TRP A | | 40.291 | 45.472 | | 1.00 20.01 | AAAA |
| MOTA | 2467 | | TRP A | | 39.165 | 43.354 | 65.202 | | |
| ATOM | 2468 | CD1 | TRP A | 310 | 38.614 | 46.938 | 65.273 | 1.00 22.82 | AAAA |
| MOTA | 2469 | NE1 | TRP A | 310 | 39.967 | 46.803 | 65.497 | 1.00 22.30 | AAAA |
| | 2470 | | TRP A | | 41.521 | 44.845 | 65.668 | 1.00 19.91 | AAAA |
| MOTA | | | | | 40.388 | 42.734 | 65.381 | 1.00 19.08 | AAAA |
| MOTA | 2471 | CZ3 | | | | | | 1.00 19.40 | AAAA |
| ATOM | 2472 | CH2 | TRP A | | 41.547 | 43.477 | 65.610 | | AAAA |
| MOTA | 2473 | С | TRP A | 310 | 36.318 | 45.279 | 67.411 | 1.00 25.26 | |
| ATOM | 2474 | 0 | TRP A | 310 | 37.262 | 44.945 | 68.109 | 1.00 24.71 | AAAA |
| ATOM | 2475 | N | CYS A | 311 | 35.467 | 46.247. | 67.749 | 1.00 26.76 | AAAA |
| | | CA | CYS A | | 35.608 | 46.975 | 69.007 | 1.00 27.89 | AAAA |
| MOTA | 2476 | | | | 34.548 | 48.081 | 69.113 | 1.00 28.98 | AAAA |
| MOTA | .2477 | CB | CYS A | | | | 67.991 | 1.00 31.89 | AAAA |
| MOTA | 2478 | SG | CYS A | | 34.798 | 49.462 | | 1.00 27.51 | AAAA |
| ATOM | 2479 | С | CYS A | 311 | 35.495 | 46.043 | 70.212 | | |
| ATOM | 2480 | 0 | CYS A | 311 | 36.289 | 46.127 | 71.135 | 1.00 26.90 | AAAA |
| ATOM | 2481 | N | GLU A | 312 | 34.495 | 45.169 | 70.187 | 1.00 27.33 | AAAA |
| | | CA | GLU A | | 34.246 | 44.210 | 71.250 | 1.00 28.03 | AAAA |
| MOTA | 2482 | | GLU A | | 33.106 | 43.287 | 70.850 | 1.00 28.55 | AAAA |
| ATOM | 2483 | CB | | | | 43.333 | 71.741 | 1.00 28.93 | AAAA |
| ATOM | 2484 | CG | GLU A | | 31.903 | | | 1.00 29.78 | AAAA |
| MOTA | 2485 | CD | GLU A | | 32.232 | 42.958 | 73.154 | | |
| ATOM | 2486 | OE1 | GLU A | 312 | 32.954 | 41.957 | 73.345 | 1.00 30.81 | AAAA |
| ATOM | 2487 | | GLU A | | 31.754 | 43.653 | 74.071 | 1.00 30.79 | AAAA |
| | 2488 | c | GLU A | | 35.463 | 43.357 | 71 514 | 1.00 28.91 | AAAA |
| MOTA | | | GLU A | | 35.822 | 43.110 | 72 662 | 1.00 30.57 | AAAA |
| MOTA | 2489 | 0 | | | | 42.889 | | 1.00 29.04 | AAAA |
| MOTA | 2490 | N | LEU A | | 36.081 | | | 1.00 28.87 | AAAA |
| MOTA | 2491 | CA | LEU A | 313 | 37.266 | 42.045 | 70.516 | | |
| ATOM | 2492 | CB | LEU A | 313 | 37.524 | 41.373 | 69.157 | | AAAA |
| | 2493 | | LEU A | 313 | 36.548 | 40.311 | 68.644 | 1.00 30.32 | AAAA |
| MOTA | | CDI | LEU A | | 36.910 | 39.872 | 67.215 | 1.00 30.26 | AAAA |
| ATOM | 2494 | נעט | LDEUA | 212 | 36.582 | 39.114 | 69.593 | | AAAA |
| MOTA | 2495 | | LEU A | 313 | | | | | AAAA |
| ATOM | 2496 | С | LEU A | | 38.474 | 42.888 | | | AAAA |
| ATOM | 2497 | 0 | LEU A | 313 | 39.215 | 42.553 | 71.808 | | |
| ATOM | 2498 | N | SER A | | 38.642 | 43.986 | | | AAAA |
| | | CA | SER A | | 39.736 | 44.927 | | 1.00 28.62 | AAAA |
| ATOM | 2499 | | SER A | | 39.690 | 45,937 | | | AAAA |
| MOTA | 2500 | CB | | | | | | | AAAA |
| ATOM | 2501 | OG | SER A | | 40.703 | 46.904 | | | AAAA |
| MOTA | 2502 | С | SER A | | 39.666 | 45.653 | | _ | |
| ATOM | 2503 | 0 | SER A | 314 | 40.488 | 46.517 | | 1.00 29.00 | AAAA |
| | 2504 | N | GLY A | 315 | 38.676 | 45.302 | 72.538 | | AAAA |
| MOTA | _ | | GLY A | | 38.535 | 45.935 | | 1.00 32.92 | AAAA |
| MOTA | 2505 | CA | | | _ | 47.452 | | | AAAA |
| ATOM | 2506 | С | GLY A | | 38.542 | | | | AAAA |
| ATOM | 2507 | 0 | GLY A | | 39.142 | 48.091 | | | |
| MOTE | 2508 | N | ARG A | 316 | 37.881 | 48.041 | . 72.794 | T.00 20.88 | AAAA. |

| ATOM | 2509 | CA | ARG . | A 316 | 37.841 | 49.493 | 72,702 | 1.00 39.49 | 7777 |
|--------|--------------|------|---------|-------|------------------|--------|--------|------------|--------|
| ATOM | 2510 | | | A 316 | 38.608 | 49.968 | 71.484 | 1.00 39.86 | AAAA |
| ATOM | 2511 | | | A 316 | 37.946 | 49.677 | 70.161 | 1.00 40.77 | |
| MOTA | 2512 | CD | | A 316 | 38.843 | 50.226 | 69.077 | 1.00 40.77 | |
| ATOM | 2513 | NE | | À 316 | 40.140 | 49.566 | 69.092 | | |
| MOTA | 2514 | CZ | | A 316 | 41.224 | | | 1.00 42.36 | |
| MOTA | 2515 | | L ARG | | | 50.057 | 68.515 | 1.00 43.38 | |
| ATOM | 2516 | NHZ | | A 316 | 41.159 42.361 | 51.217 | 67.882 | 1.00 44.76 | |
| | 2517 | C | | | | 49.385 | 68.556 | 1.00 43.71 | |
| ATOM | | | | A 316 | 36.418 | 50.015 | 72.631 | 1.00 41.54 | |
| MOTA | 2518 | 0 | | A 316 | 35.564 | 49.429 | 71.959 | 1.00 42.64 | |
| MOTA | 2519 | N | | A 317 | 36.163 | 51.119 | 73.329 | 1.00 43.10 | |
| ATOM | 2520 | CA | | A 317 | 34.830 | 51.720 | 73.356 | 1.00 44.51 | |
| ATOM | 2521 | CB | | A 317 | 34.809 | 52.936 | 74.293 | 1.00 46.17 | |
| ATOM | 2522 | CG | | A 317 | 34.472 | 52.614 | 75.759 | 1.00 49.65 | |
| ATOM | 2523 | CD | | 317 | 35.426 | 51.623 | 76.439 | 1.00 52.51 | |
| ATOM | 2524 | | . GLU I | | 35.153 | 51.251 | 77.607 | 1.00 53.37 | AAAA |
| ATOM | 2525 | OE2 | | A 317 | 36.444 | 51.214 | 75.831 | 1.00 54.14 | |
| MOTA | 2526 | C | | A 317 | 34.318 | 52.098 | 71.974 | 1.00 43.86 | AAAA |
| ATOM | 2527 | 0 | | A 317 | 35.067 | 52.532 | 71.108 | 1.00 42.46 | AAAA |
| ATOM | 2528 | N | | 4 318 | 33.023 | 51.916 | 71.779 | 1.00 44.79 | AAAA |
| ATOM | 2529 | CA | | 1 318 | 32.394 | 52.197 | 70.502 | 1.00 45.57 | AAAA |
| ATOM | 2530 | CB | VAL A | | 31.098 | 51.369 | 70.324 | 1.00 45.36 | AAAA |
| MOTA | 2531 | CG1 | VAL A | 318 | 30.537 | 51.558 | 68.924 | 1.00 45.44 | AAAA |
| MOTA | 2532 | | VAL A | | 31.366 | 49.911 | 70.612 | 1.00 46.35 | AAAA |
| MOTA | 2533 | С | VAL A | 318 | 32.007 | 53.652 | 70.377 | 1.00 46.41 | AAAA |
| ATOM | 2534 | 0 | VAL | 318 | 31.199 | 54.145 | 71.165 | 1.00 46.53 | AAAA |
| MOTA | 2535 | N | PRO A | | 32.584 | 54.370 | 69.396 | 1.00 46.89 | AAAA |
| MOTA | 2536 | CD | PRO A | 319 | 33.581 | 54.017 | 68.375 | 1.00 46.44 | AAAA |
| ATOM | 25 37 | · CA | PRO A | 319 | 32.209 | 55.774 | 69.247 | 1.00 47.62 | AAAA |
| MOTA | 2538 | CB | PRO A | 319 | 33.022 | 56.206 | 68.024 | 1.00 46.96 | AAAA |
| MOTA | 2539 | CG | PRO A | 319 | 33.161 | 54.922 | 67.251 | 1.00 46.38 | AAAA |
| MOTA | 2540 | С | PRO A | 319 | 30.709 | 55.743 | 68.977 | 1.00 48.64 | AAAA |
| MOTA | 2541 | 0 | PRO A | 319 | 30.236 | 54.860 | 68.262 | 1.00 48.61 | AAAA |
| MOTA | 2542 | N | GLU A | 320 | 29.944 | 56.667 | 69.544 | 1.00 49.24 | AAAA |
| ATOM | 2543 | CA | GLU A | 320 | 28.522 | 56.598 | 69.288 | 1.00 50.01 | AAAA |
| MOTA | 2544 | CB | GLU A | 320 | 27.720 | 57.330 | 70.363 | 1.00 51.15 | AAAA |
| MOTA | 2545 | CG | GLU A | 320 | 27.828 | 58.831 | 70.339 | 1.00 53.01 | AAAA |
| MOTA | 2546 | CD | GLU A | 320 | 26.825 | 59.474 | 71.282 | 1.00 54.34 | AAAA |
| MOTA | 2547 | OE1 | GLU A | 320 | 25.604 | 59.273 | 71.077 | 1.00 54.04 | AAAA |
| MOTA | 2548 | OE2 | GLU A | 320 | 27.255 | 60.171 | 72.228 | 1.00 55.06 | AAAA |
| MOTA | 2549 | С | GLU A | 320 | 28.206 | 57.168 | 67.921 | 1.00 49.78 | AAAA |
| MOTA | 2550 | 0 | GLU A | 320 | 27.170 | 56.861 | 67.324 | 1.00 49.79 | AAAA |
| MOTA | 2551 | N | LÝS A | 321 | 29.116 | 57.980 | 67.407 | 1.00 49.26 | AAAA |
| MOTA | 2552 | CA | LYS A | 321 | 28.906 | 58.589 | 66.109 | 1.00 49.20 | . AAAA |
| ATOM | 2553 | CB | LYS A | 321 | 28.873 | 60.106 | 66.251 | 1.00 50.38 | AAAA |
| MOTA | > 354 | CG | LYS A | 321 | 30.234 | 60.674 | 66.634 | 1.00 52.88 | AAAA |
| ATOM | 555 | CD | LYS A | 321 | 30.717 | 60.180 | 68.002 | 1.00 53.76 | AAAA |
| MOTA | 2356 | CE | LYS A | 321 | 32.229 | 60.348 | 68.154 | 1.00 55.00 | AAAA |
| ATOM | 2557 | NZ | LYS A | 321 | 32.715 | 61.725 | 67.829 | 1.00 55.95 | AAAA |
| ATOM | 2558 | С | LYS A | 321 | 30.037 | 58.207 | 65.171 | 1.00 48.64 | AAAA |
| MOTA | 2559 | 0. | LYS A | | 31.052 | 57.650 | 65.590 | 1.00 48.58 | AAAA |
| MOTA | 2560 | N | LEU A | 322 | 29.854 | 58.511 | 63.894 | 1.00 47.78 | AAAA |
| MOTA | 2561 | CA | LEU A | | 30.870 | 58.238 | 62.896 | 1.00 46.13 | AAAA |
| ATOM | 2562 | CB | LEU A | | 30.248 | 57.638 | 61.638 | 1.00 46.84 | AAAA |
| ATOM | 2563 | CG | LEU A | | 29.240 | 56.504 | 61.848 | 1.00 47.71 | AAAA |
| MOTA | 2564 | | LEU A | | 28.788 | 55.998 | 60.491 | 1.00 48.02 | AAAA |
| MOTA | 2565 | | LEU A | | 29.853 | 55.374 | 62.667 | 1.00 48.21 | |
| ATOM | 2566 | c | LEU A | | 31.427 | 59.608 | 62.580 | 1.00 44.61 | AAAA |
| ATOM | 2567 | ò | LEU A | | 30.674 | 60.571 | 62.380 | 1.00 44.61 | AAAA |
| ATOM | 2568 | N | ASN A | | 32.741 | 59.706 | | | AAAA |
| ATOM | 2569 | CA | ASN A | | 33.360 | | 62.447 | 1.00 42.66 | |
| ATOM | 2570 | СВ | ASN A | | | 60.976 | 62.135 | 1.00 41.19 | AAAA |
| ATOM | 2571 | CG | ASN A | | 34.860 35.576 | 60.904 | 62.402 | 1.00 41.07 | AAAA |
| ATOM · | 2572 | | ASN A | | | 60.001 | 61.436 | 1.00 41.43 | AAAA |
| | 2573 | | | | 35.117 | 58.901 | 61.147 | 1.00 42.46 | AAAA |
| ATOM | 2574 | | ASN A | | 36.720 | 60.449 | 60.943 | 1.00 41.77 | AAAA |
| ATOM | 2314 | С | ASN A | 323 | 33.068 | 61.223 | 60.658 | 1.00 40.76 | AAAA |

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| | | _ | | | 222 | 32.430 | ے ۔ | 0.395 | 60.010 | 1 00 | 40.19 | AAAA |
|-------|--------|-----|-------|----------|-------|---------|-----|---------|--------|------|---------|------|
| MOTA | 2575 | 0 . | ASN | | | | | 2.352 | 60.129 | | 40.11 | AAAA |
| MOTA | 2576 | N | ASN | | | 33.523 | | | | | 39.99 | AAAA |
| ATOM | 2577 | CA | ASN | | | 33.268 | | 2.699 | 58.735 | | | |
| ATOM | 2578 | CB | ASN | Α | 324 | 33.711 | | 4.128 | 58.472 | | 39.54 | AAAA |
| ATOM | 2579 | CG | ASN | Α | 324 | 33.003 | 6 | 5.114 | 59.361 | | 40.88 | AAAA |
| ATOM | 2580 | OD1 | ASN | A | 324 | 31.763 | 6 | 5.145 | 59.417 | | 40.77 | AAAA |
| ATOM | 2581 | ND2 | ASN | Α | 324 | 33.779 | 6 | 5.938 | 60.064 | | 40.63 | AAAA |
| | 2582 | Ċ. | | | 324 | 33.918 | 6 | 1.786 | 57.712 | 1.00 | 40.10 | AAAA |
| MOTA | | ō | ASN | | | 33.320 | _ | 1.468 | 56.678 | 1.00 | 39.24 | AAAA |
| ATOM | 2583 | | | | | 35.144 | | 1.376 | 58.011 | 1.00 | 40.41 | ÁAAA |
| MOTA | 2584 | N | LYS | | | | | 0.519 | 57.126 | | 41.41 | AAAA |
| MOTA | 2585 | CA | LYS | | | 35.908 | | | 57.761 | | 42.64 | AAAA |
| MOTA | 2586 | CB | LYS | | | 37.262 | | 0.201 | | | 44.45 | AAAA |
| ATOM | 2587 | CG | LYS | | | 38.224 | | 9.504 | 56.828 | | | AAAA |
| MOTA | 2588 | CD | LYS | | | 39.575 | | 9.199 | 57.491 | | 45.61 | |
| MOTA | 2589 | CE | LYS | Α | 325 | 40.358 | | 0.464 | 57.850 | | 45.88 | AAAA |
| ATOM | 2590 | NZ | LYS | | | 41.717 | | 0.151 | 58.494 | | 46.27 | AAAA |
| ATOM | 2591 | С | LYS | Α | 325 | 35,124 | 5 | 9.248 | 56.856 | | 41.56 | AAAA |
| ATOM | 2592 | 0 | | | 325 | 35,042 | : 5 | 8.781 | 55.716 | | 41.35 | AAAA |
| | 2593 | N | | | 326 | 34.524 | 1 5 | 8.703 | 57.906 | 1.00 | 41.32 | AAAA |
| MOTA | 2594 | CA | | | 326 | 33.732 | | 7.492 | 57.774 | 1.00 | 41.07 | AAAA |
| ATOM | | CB | | | 326 | 33.452 | | 6.912 | 59.143 | 1.00 | 40.87 | AAAA |
| MOTA | 2595 | | | | 326 | 32.420 | | 7.722 | 57.019 | 1.00 | 41.24 | AAAA |
| MOTA | 2596 | С | | | | 32.045 | | 6.913 | 56.174 | | 40.91 | AAAA |
| ATOM | 2597 | 0 | | | 326 | | | 8.815 | 57.316 | | 41.92 | AAAA |
| MOTA | 2598 | N | | | 327 | 31.719 | | | 56.631 | | 42.20 | AAAA |
| ATOM | 2599 | CA | | | 327 | 30.451 | | 9.097 | | | 43.61 | AAAA |
| MOTA | 2600 | CB | .LYS | | | 29.796 | | 50.374 | 57.170 | | - | AAAA |
| ATOM | 2601 | CG | | | 327 | 29.534 | | 50.413 | 58,670 | | 45.83 | |
| ATOM | 2602 | CD | LYS | A | 327 · | 28.745 | | 51.681 | 59.029 | | 47.34 | AAAA |
| MOTA | 2603 | CE. | LYS | Α | 327 | 28.682 | | 51.952 | 60.538 | | 48.28 | AAAA |
| ATOM | 2604 | NZ | LYS | A | 327 | 28.090 | 0 (| 50.845 | 61.351 | | 48.98 | AAAA |
| ATOM | 2605 | С | LYS | Α | 327 | 30.673 | 3 5 | 59.266 | 55.125 | | 41.33 | AAAA |
| ATOM | 2606 | ŏ | | | 327 | 29.879 | 9 ! | 58.797 | 54.309 | | 40.78 | AAAA |
| | 2607 | N | | | 328 | 31,76 | 1 ! | 59.950 | 54.781 | | 40.39 | AAAA |
| MOTA | 2608 | CA | | | 328 | 32.12 | | 60.217 | 53.399 | | 38.91 | AAAA |
| ATOM | 2609 | CB | | | 328 | 33.30 | | 61.199 | 53.369 | 1.00 | 40.04 | AAAA |
| ATOM | | CG | | | 328 | 32.94 | | 62.576 | 53.909 | 1.00 | 41.94 | AAAA |
| MOTA | 2610 | | | | 328 | 34.13 | | 63.515 | 53.994 | 1.00 | 43.77 | AAAA |
| ATOM | 2611 | CD | GLU | | | 34.90 | | 63.595 | 53.010 | 1.00 | 44.29 | AAAA |
| ATOM | 2612 | OEI | GLU | , A | 320 | 34.28 | | 64.189 | 55.040 | 1.00 | 45.11 | AAAA |
| MOTA | 2613 | | | | | 32.49 | | 58.938 | 52.675 | | 37.39 | AAAA |
| MOTA | 2614 | C | | | 328 | 32.11 | | 58.722 | 51.525 | | 37.31 | AAAA |
| ATOM | 2615 | 0 | | | 328 | | | | 53.355 | | 35.67 | AAAA |
| MOTA | 2616 | N | | | 329 | 33.25 | | 58.091 | 52.783 | | 33.03 | AAAA |
| ATOM | 2617 | CA | | | 329 | 33.65 | | 56.820 | | | 30.62 | AAAA |
| ATOM | 2618 | CB | | | . 329 | 34.45 | | 56.012 | 53.813 | | 0 27.48 | AAAA |
| ATOM | 2619 | CG | | | 329 | 34.76 | | 54.549 | 53.481 | | | |
| ATOM | 2620 | CDI | LEU | Α | 329 | 35.54 | | 54.453 | 52.193 | | 0 36.24 | AAAA |
| ATOM | 2621 | CD2 | LEU | A | 329 | 35.51 | 4 | 53.936 | 54.622 | | 0 25.74 | AAAA |
| ATOM | 2622 | С | | | 329 | 32.40 | | 56.057 | 52.368 | | 0 33.24 | AAAA |
| ATOM | 2623 | ō | | | 329 | 32.23 | 9 | 55.708 | 51.205 | | 0 32.72 | AAAA |
| | 2624 | N | | | 330 | 31.51 | | 55.810 | 53.327 | 1.0 | 0 33.92 | AAAA |
| MOTA | | CA | | | 330 | 30.28 | | 55.090 | 53.046 | | 0 34.91 | AAAA |
| MOTA | 2625 | CB | | | 330 | 29.41 | 1 | 55.023 | 54.292 | 1.0 | 0 34.02 | AAAA |
| ATOM | 2626 | | TEN | ים וא | 330 | 30.06 | | 54.236 | | | 0 34.06 | AAAA |
| MOTA | 2627 | CG | 2 577 | | 330 | 29.09 | | 54.060 | | 1.0 | 0 33.63 | AAAA |
| MOTA | . 2628 | נט | LEU | | 330 | 30.51 | | 52.892 | | | 0 33.82 | AAAA |
| MOTA | 2629 | | LEU | | 330 | | | 55.695 | | | 0 35.94 | AAAA |
| MOTA | 2630 | С | | | 330 | 29.49 | | | | | 0 36.14 | AAAA |
| ATOM | 2631 | 0 | | | 330 | 28.98 | | 54.968 | | | 0 38:17 | AAAA |
| MOTA | 2632 | И | | | 331 | 29.41 | | 57.022 | 51.883 | | 0 41.05 | AAAA |
| ATOM | 2633 | CA | | | 331 | 28.66 | | 57.718 | | | | |
| ATOM | 2634 | CB | LYS | 5 2 | 331 | - 28.40 |)7 | 59.161 | | | 0 41.83 | AAAA |
| MOTA | 2635 | CG | | | 331 | 27.58 | 34 | 59.358 | | | 0 43.26 | AAAA |
| MOTA | 2636 | CD | | | 331 | 27.20 |)2 | 60.823 | | | 0 44.15 | AAAA |
| | 2637 | CE | | | 331 | 26.18 | | 61.333 | | 1.0 | 0 45.71 | AAAA |
| ATOM | | | | | 331 | 25.69 | | 62.735 | | 1.0 | 0 45.95 | AAAA |
| MOTA | 2638 | _ | | | 331 | 29.34 | | 57.681 | | 1.0 | 0 42.22 | AAAA |
| MOTA | 2639 | | | | 331 | 28.71 | | | 48.480 | | 0 41.94 | AAAA |
| ATOM | 2640 | ٠. | 2025 | | | 20.73 | | | - | | | • |
| • • • | | • | | | | | | | | | | |

| ATOM' | 2641 | 1/3 | SER A 332 | 30.618 | F7 316 | 40 460 | | |
|--------|------|-----|--------------------|--------|--------|--------|------------|--------|
| | | N. | | | 57.316 | 49.463 | 1.00 44.45 | AAAA |
| MOTA | 2642 | CA | S <u>E</u> R A 332 | 31.351 | 57.271 | 48.202 | 1.00 46.88 | AAAA |
| MOTA | 2643 | CB | SER A 332 | 32.854 | 57.416 | 48.435 | 1.00 46.49 | AAAA |
| MOTA | 2644 | OG | SER A 332 | 33.380 | 56.263 | 49.058 | 1.00 45.65 | AAAA |
| MOTA | 2645 | С | SER A 332 | 31.093 | 55.959 | 47.494 | 1.00 48.73 | |
| ATOM - | 2646 | ō | SER A 332 | | | | | AAAA |
| | | | | 31.262 | 55.854 | 46.281 | 1.00 49.51 | AAAA |
| ATOM | 2647 | N | ILE A 333 | 30.697 | 54.952 | 48.258 | 1.00 50.62 | AAAA |
| MOTA | 2648 | CA | ILE A 333 | 30.420 | 53.648 | 47.686 | 1.00 52.65 | AAAA |
| MOTA | 2649 | CB | ILE A.333 | 30.246 | 52.584 | 48.779 | 1.00 52.35 | AAAA |
| ATOM | 2650 | CG2 | ILE A 333 | 29.889 | 51.248 | 48.157 | 1.00 51.40 | |
| ATOM | 2651 | | ILE A 333 | 31.522 | | | | AAAA |
| | | | | | 52.465 | 49.596 | 1.00 52.29 | AAAA |
| ATOM | 2652 | | ILE A 333 | 31.403 | 51.463 | | 1.00 53.23 | AAAA |
| MOTA | 2653 | С | ILE A 333 | 29.120 | 53.712 | 46.924 | 1.00 54.42 | AAAA |
| ATOM _ | 2654 | 0 | ILE A 333 | 28.122 | 54.178 | 47.462 | 1.00 55.10 | AAAA |
| MOTA | 2655 | N | ASP A 334 | 29.118 | 53.274 | 45.672 | 1.00 56.56 | AAAA |
| ATOM | 2656 | CA | ASP A 334 | 27.863 | 53.263 | 44.940 | 1.00 59.13 | - AAAA |
| ATOM | 2657 | СВ | ASP A 334 | 28.050 | 53.460 | 43.433 | | |
| | 2658 | CG | ASP A 334 | | | | | AAAA |
| ATOM | | | | 28.976 | 52.446 | 42.823 | 1.00 59.23 | AAAA |
| ATOM | 2659 | | ASP A 334 | 28.853 | 52.194 | 41.606 | 1.00 58.87 | AAAA |
| MOTA | 2660 | OD2 | ASP A 334 | 29.839 | 51.925 | 43.559 | 1.00 59.34 | AAAA |
| MOTA | 2661 | С | ASP A 334 | 27.251 | 51.898 | 45.215 | 1.00 60.95 | AAAA |
| MOTA | 2662 | Ó | ASP A 334 | 27.803 | 50.861 | 44.840 | 1.00 61.15 | AAAA |
| ATOM | 2663 | N | PHE A 335 | 26.113 | 51.914 | 45.897 | 1.00 62.56 | |
| MOTA | 2664 | CA | PHE A 335 | | • | | | AAAA |
| | | | | 25.414 | 50.701 | 46.257 | 1.00 64.12 | AAAA |
| ATOM . | 2665 | CB | PHE A 335 | 25.311 | 50.621 | 47.779 | 1.00 64.40 | AAAA |
| MOTA | 2666 | CG | PHE A 335 | 24.224 | 49.714 | 48.263 | 1.00 64.98 | AAAA |
| ATOM | 2667 | CD1 | PHE A 335 | 24.180 | 48.379 | 47.868 | 1.00 65.54 | AAAA |
| MOTA | 2668 | CD2 | PHE A 335 | 23.234 | 50.197 | 49.107 | 1.00 65.12 | AAAA |
| MOTA | 2669 | CE1 | PHE A 335 | 23.163 | 47.539 | 48.305 | 1.00 65.75 | AAAA |
| ATOM | 2670 | | PHE A 335 | 22.213 | 49.367 | 49.552 | 1.00 65.79 | |
| ATOM | 2671 | CZ | PHE A 335 | 22.177 | | | | AAAA |
| | | | | | 48.034 | 49.150 | 1.00 66.01 | AAAA |
| MOTA | 2672 | C | PHE A 335 | 24.025 | 50.626 | 45.640 | 1.00 65.41 | AAAA |
| ATOM | 2673 | 0 | PHE A 335 | 23.591 | 49.564 | 45.184 | 1.00 65.27 | AAAA |
| MOTA | 2674 | N | GLU A 336 | 23.338 | 51.763 | 45.618 | 1.00 66.38 | AAAA |
| MOTA | 2675 | CA | GLU A 336 | 21.980 | 51.826 | 45.097 | 1.00 67.49 | AAAA |
| MOTA | 2676 | CB | GLU A 336 | 21.893 | 51.26Ò | 43.673 | 1.00 68.25 | AAAA |
| MOTA | 2677 | CG | GLU A 336 | 20.459 | 51.230 | 43.116 | 1.00 69.15 | AAAA |
| ATOM | 2678 | CD | GLU A 336 | 20.334 | 50.465 | 41.804 | 1.00 69.40 | |
| ATOM | 2679 | | GLU A 336 | 20.710 | • | | | AAAA |
| | | | | | 49.271 | 41.784 | 1.00 69.57 | AAAA |
| ATOM | 2680 | | GLU A 336 | 19.851 | 51.051 | 40.804 | 1.00 69.10 | Aaaa |
| ATOM | 2681 | С | GLU A 336 | 21.098 | 50.999 | 46.025 | 1.00 67.68 | AAAA |
| MOTA | 2682 | 0 | GLU A 336 | 21.216 | 49.776 | 46.082 | 1.00 67.58 | AAAA |
| ATOM | 2683 | N | GLU A 337 | 20.227 | 51.679 | 46.761 | 1.00 67.87 | AAAA |
| MOTA | 2684 | CA | GLU A 337 | 19.317 | 51.020 | 47.686 | 1.00 68.66 | AAAA |
| ATOM | 2685 | CB | GLU A 337 | 18.583 | 52.085 | 48.502 | 1.00 68.88 | AAAA |
| ATOM | 2686 | CG | GLU : 337 | 18.279 | 51.715 | 49.944 | | |
| MOTA | 2687 | CD | GLU A 337 | | | | | AAAA |
| | | | •• | 19.527 | 51.587 | 50.789 | 1.00 67.70 | AAAA |
| ATOM | 2688 | | GLU 337 | 20.319 | 52.554 | 50.851 | 1.00 67.05 | AAAA |
| MOTA | 2689 | OE2 | GLU A 337 | 19.711 | 50.518 | 51.398 | 1.00 67.79 | AAAA |
| MOTA | 2690 | C | GLU A 337 | 18.322 | 50.222 | 46.827 | 1.00 69.28 | AAAA |
| ATOM | 2691 | 0 | GLU A 337 | 17.886 | 50.705 | 45.780 | 1.00 69.50 | AAAA |
| ATOM | 2692 | N | PHE A 338 | 17.966 | 49.012 | 47.259 | 1.00 69.55 | AAAA |
| MOTA | 2693 | CA | PHE A 338 | 17.035 | 48.176 | 46.497 | 1.00 69.67 | |
| | 2694 | | PHE A 338 | | | | | AAAA |
| MOTA | | CB | | 16.995 | 46.759 | 47.066 | 1.00 70.51 | A'AAA |
| ATOM | 2695 | CG | PHE A 338 | 16.225 | 45.789 | 46.221 | 1.00 71.57 | AAAA |
| MOTA | 2696 | CD1 | PHE A 338 | 16.666 | 45.462 | 44.936 | 1.00 72.04 | AAAA |
| MOTA | 2697 | CD2 | PHE A 338 | 15.052 | 45.208 | 46.698 | 1.00 71.69 | AAAA |
| MOTA | 2698 | | PHE A 338 | 15.944 | 44.566 | 44.138 | 1.00 72.23 | AAAA |
| ATOM | 2699 | | PHE A 338 | 14.323 | 44.313 | 45.909 | 1.00 71.93 | AAAA |
| ATOM | 2700 | CZ | PHE A 338 | | | | | |
| | | | | 14.770 | 43.991 | 44.627 | 1.00 72.11 | AAAA |
| ATOM | 2701 | | PHE A 338 | 15.633 | 48.770 | 46.494 | 1.00 69.26 | AAAA |
| ATOM | 2702 | | PHE A 338 | 15.072 | 49.029 | 45.434 | 1.00 68.86 | AAAA |
| MOTA | 2703 | N | ASP A 339 | 15.053 | 48.962 | 47.674 | 1.00 69.35 | AAAA |
| MOTA | 2704 | | ASP A 339 | 13.733 | 49.572 | 47.755 | 1.00 69.61 | · AAAA |
| ATOM | 2705 | | ASP A 339 | 13.134 | 49.457 | 49.157 | 1.00 69.48 | AAAA |
| MOTA | 2705 | | ASP A 339 | | | | | |
| HIOH. | 2,00 | -3 | נננ ח זשה | 11.819 | 50.233 | 49.299 | 1.00 69.72 | AAAA |

| | | | 3 CD 3 | 220 | 11.813 | . 5 | 1.462 | 49.058 | 1.00 | 69.39 | AAAA |
|---------------|--------------|---------|----------------|----------------|--------------|-----|-------------------|------------------|-------|--------------------|--------------|
| MOTA | 2707 | ODI | ASP A ASP A | 339 | 10.790 | | 9.618 | 49.655 | | 69.78 | AAAA |
| MOTA | 2708 | 002 | ASP A | 330 | 13.97 | | 1.035 | 47.440 | 1.00 | 69.95 | AAAA |
| MOTA | 2709 | C | ASP A | 339 | 14.30 | | 1.815 | 48.333 | 1.00 | 69.92 | AAAA |
| MOTA | 2710 | 0 | ASP A | 340 | 13.81 | | 1.389 | 46.168 | 1.00 | 70.23 | AAAA |
| MOTA | 2711 | N | ASP A | 340 | 14.02 | - | 52.748 | 45.699 | | 70.39 | AAAA |
| ATOM | 2712 | | ASP A | | 12.75 | | 53.283 | 45.041 | | 70.64 | AAAA |
| MOTA | 2713 | CG | ASP A | | 12.39 | | 52.517 | 43.791 | | 70.86 | AAAA |
| MOTA | 2714 | 001 | ASP A | | 12.12 | | 51.302 | 43.903 | | 70.93 | AAAA |
| MOTA | 2715 2716 | 001 | ASP A | 340 | 12.39 | | 53.125 | 42.699 | | 70.89 | AAAA |
| MOTA | 2717 | C | ASP A | | 14.48 | | 53.674 | 46.807 | | 70.63 | AAAA |
| ATOM | 2718 | ō | ASP A | | 15.68 | 8 | 53.847 | 47.008 | | 71.13 | AAAA |
| MOT'A ATOM | 2719 | Ŋ | GLU A | | 13.54 | 3 | 54.259 | 47.544 | | 69.95 | AAAA · |
| ATOM | 2720 | CA | GLU A | | 13.94 | | 55.150 | 48.619 | | 69.17 | AAAA AAAA |
| ATOM | 2721 | CB | GLU A | 341 | 13.63 | | 56.613 | 48,266 | | 70.83 | AAAA |
| ATOM | 2722 | CG | GLU A | 341 | 14.09 | _ | 57.601 | 49.347 | | 73.44 75.27 | AAAA |
| ATOM | 2723 | CD | GLU A | | 13.95 | | 59.071 | 48.951 | | 76.21 | AAAA |
| ATOM | 2724 | OE1 | GLU A | 341 | 12.82 | | 59.518 | 48.646 | | 75.69 | AAAA |
| ATOM | 2725 | OE2 | GLU A | 341 | 14.98 | - | 59.786 | 48.954 49.983 | | 67.09 | AAAA |
| ATOM | 2726 | С | GLU A | | 13.36 | | 54.819 | 50.297 | | 66.57 | AAAA |
| MOTA | 2727 | 0 | GLU A | | 12.23 | | 55.176 | | | 64.87 | AAAA |
| MOTA | 2728 | N | VAL A | | 14.15 | | 54.114. 53.779 | 52.148 | | 62.55 | AAAA |
| ATOM | 2729 | CA | VAL A | | 13.76 | | 52.377 | 52.589 | | 62.81 | AAAA |
| MOTA | 2730 | CB | VAL A | | 14.20 | | 52.193 | 54.081 | 1.00 | 62.56 | AAAA |
| MOTA | 2731 | | VAL A | | 13.53 | | 51.298 | 51.849 | 1.00 | 63.69 | AAAA |
| MOTA | 2732 | | VAL A | | 14.48 | | 54.822 | 52.982 | 1.00 | 59.94 | AAAA |
| ATOM | 2733 | C | VAL A | | 14.02 | | 55.215 | 54.054 | 1.00 | 59.91 | AAAA |
| MOTA | 2734 | 0 | ASP A | | 15.6 | | 55.278 | 52.442 | 1.00 | 56.85 | AAAA |
| MOTA | 2735 | N CA | ASP A | | 16.4 | | 56.266 | 53.085 | 1.00 | 54.01 | AAAA |
| MOTA | 2736 2737 | CB | ASP A | | 15.6 | | 57.446 | 53.605 | | 54.18 | AAAA |
| MOTA | 2738 | CG | | 343 | 16.5 | | 58.511 | 54.241 | | 53.96 | AAAA |
| MOTA | 2739 | | ASP A | | 15.9 | 47 | 59.485 | 54.785 | | 54.59 | AAAA |
| MOTA MOTA | 2740 | OD2 | ASP A | A 343 - | 17.7 | 47 | 58.373 | 54.191 | | 53.61 | AAAA AAAA |
| ATOM | 2741 | c | | A 343 | 17.1 | | 55.609 | 54.242 | | 0 51.92 | AAAA |
| ATOM | 2742 | 0 | ASP A | A 343 | 16.6 | | 55.371 | | | 0 51.89 0 48.86 | AAAA |
| MOTA | 2743 | N | ARG | A 344 | 18.4 | | 55.306 | | 1.0 | 0 45.59 | AAAA |
| ATOM | 2744 | CA | ARG A | A 344 | 19.2 | | 54.676 | | | 0 43.94 | AAAA |
| MOTA | 2745 | CB | | A 344 | 19.8 | | 53.369 52.289 | | | 0 41.70 | AAAA |
| MOTA | 2746 | CG | | A 344 | 18.8 | | 51.955 | | | 0 38.94 | AAAA |
| MOTA | 2747 | | | A 344 | 17.9 17.1 | | 50.781 | | | 0 36.78 | AAAA |
| MOTA | 2748 | | | A 344 | 16.1 | | 50.316 | | | 0 34.81 | AAAA |
| ATOM | 2749 | | ARG . | A 344 | 15.8 | | 50.927 | | 1.0 | 0 34.11 | AAAA |
| MOTA | 2750 | _ | | A 344 | 15.5 | | 49.228 | | | 0 31.84 | · AAAA |
| MOTA | 2751 | | | A 344 | 20.3 | | 55.604 | 55.520 | | 0 44.83 | AAAA |
| ATOM | 2752 2753 | | | A 344 | 21.3 | | 55.157 | | | 0 43.97 | AA A |
| MOTA | 2754 | | SER | A 345 | 20.1 | .92 | 56.895 | | | 0 44.32 | AF AA |
| MOTA MOTA | 2755 | | SER | A 345 | 21.1 | .99 | 57.877 | | | 0 43.74 | AAAA AAAA |
| ATOM | 2756 | | | A 345 | 20.8 | | 59.248 | 55.039 | | 0 44.49 | AAAA |
| ATOM | 2757 | | SER | A 345 | 19.6 | | 59.729 | | | 0 46.07 | AAAA |
| ATOM | 2758 | | SER | A 345 | 21.3 | | 57.977 | 57.144 | | 00 42.82 | AAAA |
| ATOM | 2759 | | SER | A 345 | 22.3 | 304 | 58.472 | | 1 1.6 | 0 41.48 | AAAA |
| MOTA | 2760 | N | TYR | A 346 | 20.2 | 282 | 57.509 | | 1 1 6 | 0 40.35 | AAAA |
| ATOM | 2761 | . ÇA | TYR | A 346 | 20.2 | | 57.549 | | 1 1 | 0 40.38 | AAAA |
| ATOM | 2762 | | TYR | A 346 | 18.9 | | 57.068 55.603 | | | 0 39.28 | AAAA |
| MOTA | 2763 | | TYR | A 346 | 18.0 | | 54.58 | | 5 1.6 | 00 38.74 | AAAA |
| MOTA | 2764 | | 1 TYR | A 346 | 19.7 19.0 | | 53.24 | | | 00 37.71 | AAAA |
| ATOM | 2765 | | 1 TYR | A 340 | 17. | | 55.22 | | 3 1.0 | 00 38.49 | AAAA |
| MOTA | 2766 | | | A 346 | 17. | | 53.88 | · | 8 1.0 | 00 38.17 | AAAA |
| ATCM | 2767 | | Z TXK | A 346 A 346 | 18. | | 52.89 | | 6 1. | 00 37.59 | AAAA |
| MOTA | | | | A 346 | 17. | | 51.58 | | 8 1. | 00 37.14 | AAAA |
| MOTA | | | | A 346 | 21. | | 56.68 | | 9 1. | 00 39.91 | AAAA |
| ATOM | | | | A 346 | 21. | 967 | 56.95 | 7 60.92 | 1 1. | 00 40.28 | AAAA |
| ATOM | | | | A 347 | | 800 | | | 3 1. | 00 39.14 | AAAA |
| ATCM | 277 | ~ 14 | | | | | | - | | | • |
| | | | _ | | | | | | | | |

| MOTA | 2773 | CA | MET | Α | 347 | 22.879 | 54.756 | 59.530 | 1.00 38.1 | AAAA e. |
|--------|------|-----|-------|-----|-----|--------|---------------------|--------|------------|---------|
| ATOM | 2774 | CB | MET | Α | 347 | 23.042 | 53.582 | 58.566 | 1.00 38.2 | |
| ATOM | 2775 | CG | _ | | 347 | | | | | _ |
| | | | | | | 21.973 | 52.523 | 58.694 | 1.00 38.1 | |
| ATOM | 2776 | SD | MET | | | 22.317 | 51.115 | 57.641 | 1.00 38.0 | S AAAA |
| MOTA | 2777 | CE | MET | Α | 347 | 22.237 | 51.892 | 56.101 | 1.00 37.6 | AAAA |
| ATOM | 2778 | C | MET | Α | 347 | 24.189 | 55.494 | 59.603 | 1.00 38.0 | |
| | 2779 | | | | | | | | | |
| ATOM | | 0 | MET | | | 25.127 | 55.033 | 60.250 | 1.00 37.4 | |
| ATOM | 2780 | N | LEU | A | 348 | 24.248 | 56.637 | 58.929 | 1,00 38.0 | AAAA 8 |
| MOTA | 2781 | CA | LEU | Α | 348 | 25.449 | 57.463 | 58.898 | 1.00 38.0 | |
| MOTA | 2782 | CB | LEU | | | 25.445 | 58.330 | 57.638 | 1.00 36.6 | |
| | | | | | | | | | | |
| MOTA | 2783 | CG | | | 348 | 25.379 | 57.583 | 56.310 | 1.00 35.4 | 7 AAAA |
| ATOM | 2784 | CD1 | LEU | Α | 348 | 25.285 | 58.559 | 55.165 | 1.00 34.5 | il aaaa |
| ATOM | 2785 | CD2 | LEU | Α | 348 | 26.605 | 56.716 | 56.167 | 1.00 36.5 | |
| MOTA | 2786 | С | LEU | | | 25.521 | 58.353 | 60.138 | | |
| | | | | | | | | | 1.00 39.0 | |
| ATOM | 2787 | 0 | LEU | | | 26.546 | 58.980 | 60.406 | 1.00 38.8 | |
| MOTA | 2788 | И. | GLU | A | 349 | 24.432 | 58.385 | 60.898 | 1.00 39.9 | AAAA 0 |
| ATOM | 2789 | CA | GLU | A | 349 | 24.363 | 59.213 | 62.092 | 1.00 40.9 | |
| MOTA | 2790 | CB | CLII | A | 349 | 22.961 | 59.821 | 62.203 | 1.00 41.7 | |
| | | | | | * | | | | | |
| ATOM | 2791 | CG | GLU | | | 22.515 | 60.629 | 60.966 | 1.00 42.2 | |
| ATOM | 2792 | CD | GLU | Α | 349 | 23.349 | 61.891 | 60.708 | 1.00 42.5 | 1 AAAA |
| MOTA | 2793 | OE1 | GLU | Α | 349 | 23.414 | 62.778 | 61.587 | 1.00 42.3 | |
| ATOM | 2794 | | GLU | | | 23.933 | 61.998 | 59.614 | 1.00 43.3 | |
| | | | | | | | | | | |
| ATOM | 2795 | C | GLU | | | 24.740 | 58.511 | 63.406 | 1.00 41.1 | |
| ATOM | 2796 | О | GLU | | | 24.664 | 59.118 | 64.476 | 1.00 41.3 | AAAA 8 |
| MOTA | 2797 | N | THR | Α | 350 | 25.140 | 57.243 | 63.326 | 1.00 40.8 | |
| ATOM | 2798 | CA | THR | Α | 350 | 25.555 | 56.475 | 64.504 | 1.00 40.6 | |
| ATOM | 2799 | CB | THR | | | 24.405 | 56.283 | | | |
| | | | | | | | | 65.510 | 1.00 41.5 | |
| ATCM | 2800 | | THR | | | 24.062 | 57.549 | 66.078 | 1.00 41.4 | AAAA 8 |
| MOTA | 2801 | CG2 | THR | А | 350 | 24.821 | 55.345 | 66.638 | 1.00 41.1 | .9 AAAA |
| ATOM | 2802 | С | THR | Α | 350 | 26.109 | 55.109 | 64.141 | 1.00 40.1 | |
| ATOM | 2803 | 0 | THR | | | 25.857 | 54.595 | 63.055 | 1.00 39.9 | |
| | | | | | | | | | | |
| ATOM | 2804 | N | LEU | | | 26.865 | 54.527 | 65.067 | 1.00 40.3 | |
| ATOM | 2805 | CA | LEU | | | 27.491 | 53.227 _. | 64.857 | 1.00 40.7 | AAAA 0' |
| ATOM | 2806 | CB | LEU | Α | 351 | 28.855 | 53.213 | 65.540 | 1.00 39.8 | 9 AAAA |
| ATOM | 2807 | CG | LEU | А | 351 | 29.911 | 52.290 | 64.951 | 1.00 39.6 | |
| ATOM | 2808 | | LEU | | | 31.170 | 52.403 | 65.772 | | |
| | | | | | | | | | 1.00 39.8 | |
| MOTA | 2809 | | LEU | | | 29.414 | 50.861 | 64.945 | 1.00 40.7 | AAAA 0' |
| MOTA | 2810 | С | LEU | Α | 351 | 26.612 | 52.091 | 65.384 | 1.00 41.1 | .2 AAAA |
| ATOM | 2811 | 0 | LEU | Α | 351 | 26.467 | 51.060 | 64.736 | 1.00 40.0 | 2 AAAA |
| ATOM | 2812 | N | LYS | | | 26.040 | 52.292 | 66.567 | 1.00 42.9 | |
| ATOM | 2813 | CA | LYS | | | | | | | |
| | | | | | | 25.138 | 51.326 | 67.201 | 1.00 43.9 | |
| ATCM | 2814 | CB | LYS | | | 25.412 | 51.225 | 68.707 | 1.00 43.3 | AAAA 8 |
| . ATOM | 2815 | CG | LYS | Α | 352 | 26.743 | 50.597 | 69.055 | 1.00 44.6 | AAAA 8 |
| MOTA | 2816 | CD | LYS | Α | 352 | 27.185 | 50.927 | 70.482 | 1.00 45.4 | AAAA 8 |
| ATOM | 2817 | CE | LYS | | | 26.189 | 50.500 | 71.539 | 1.00 46.2 | |
| | | | | | | | | | | |
| ATOM | 2818 | NZ | LYS | | | 76.646 | 50.944 | 72.895 | 1.00 47.3 | |
| MOTA | 2819 | С | LYS | A | 352 | 23.723 | 51.838 | 67.003 | 1.00 44.4 | AAAA 0 |
| ATOM | 2820 | 0 | LYS | A | 352 | 23.375 | 52.917 | 67.488 | 1.00 45.7 | 9 AAAA |
| ATOM | 2821 | N | ASP | А | 353 | 22.904 | 51.083 | 66.287 | 1.00 44.7 | |
| ATOM | 2822 | CA | ASP | | | 21.532 | | | | |
| | | | | | | | 51.509 | 66.074 | 1.00 44.7 | |
| ATOM | 2823 | CB | ASP | A | 353 | 21.050 | 51.030 | 64.702 | 1.00 45.2 | AAAA 0: |
| ATOM | 2824 | CG | ASP | A | 353 | 21.146 | 49.544 | 64.546 | .1.00 45.2 | 1 AAAA |
| ATOM | 2825 | OD1 | ASP | А | 353 | 21.806 | 49.086 | 63.581 | 1.00 45.0 | |
| MOTA | 2826 | | ASP | | | 20.549 | | | | |
| | | | | | | | 48.841 | 65.391 | 1.00 45.5 | |
| MOTA | 2827 | C | ASP . | | | 20.645 | 50.993 | 67.217 | 1.00 44.4 | 4 AAAA |
| ATCM | 2828 | 0 | ASP . | A | 353 | 21.042 | 50.113 | 67.973 | 1.00 44.2 | 9 AAAA |
| ATOM | 2829 | N | PRO . | | | 19.439 | 51.553 | 67.367 | 1.00 44.2 | |
| | 2830 | | PRO | | | 18.839 | _ | | | |
| ATOM | | CD | | | | | 52.617 | 66.550 | 1.00 44.3 | |
| ATCM | 2831 | CA | PRO . | | | 18.500 | 51.163 | 68.419 | 1.00 44.1 | AAAA 8. |
| ATCM | 2832 | CB | PRO . | A | 354 | 17.371 | 52.170 | 68.238 | 1.00 44.5 | 2 AAAA |
| ATCM | 2833 | CG | PRO . | | | 17.368 | 52.341 | 66.749 | 1.00 44.6 | |
| ATOM | 2834 | | PRO . | | | 17.995 | | | | |
| | | C | | | | | 49.740 | 68.328 | 1.00 43.8 | |
| ATOM | 2835 | 0 | PRO . | | | 17.962 | 49.152 | 67.249 | 1.00 44.4 | |
| ATCM . | 2836 | И | TRP . | A | 355 | 17.588 | 49.198 | 69.469 | 1.00 43.2 | AAAA E |
| ATOM | 2837 | CA | TRP | A | 355 | 17.051 | 47.851 | 69.500 | 1.00 42.8 | |
| ATCH | 2838 | CB | TRP | | | 16.743 | 47.401 | 70.927 | 1.00 46.4 | |
| ALCIA. | 2030 | -13 | . The | • • | | 20.743 | 31.30T | 10.321 | ¥.00 90.4 | AMAM. |

| ATOM 2839 CG TRP À 355 17.959 47.052 11.893 1.00 52.56 AAAA ATOM 2841 CEZ TRP À 355 19.684 45.868 71.879 1.00 52.203 AAAA ATOM 2842 CEZ TRP À 355 19.684 45.868 71.879 1.00 52.203 AAAA ATOM 2843 CDJ TRP À 355 18.036 44.77.308 72.846 1.00 52.25 AAAA ATOM 2844 NEI TRP À 355 18.036 44.77.308 72.846 1.00 51.63 AAAA ATOM 2845 CZZ TRP À 355 18.036 44.77.308 72.846 1.00 51.63 AAAA ATOM 2845 CZZ TRP À 355 20.008 43.518 72.846 1.00 51.63 AAAA ATOM 2846 CZZ TRP À 355 20.008 43.518 72.846 1.00 51.63 AAAA ATOM 2846 CZZ TRP À 355 20.008 43.518 72.846 1.00 51.63 AAAA ATOM 2846 CZZ TRP À 355 20.008 43.518 72.846 1.00 51.63 AAAA ATOM 2846 CZZ TRP À 355 15.798 47.767 68.675 1.00 40.28 AAAA ATOM 2848 CZ TRP À 355 15.798 47.767 68.675 1.00 40.28 AAAA ATOM 2848 CZ TRP À 355 15.798 47.767 68.675 1.00 40.28 AAAA ATOM 2848 C TRP À 355 15.074 48.700 68.065 1.00 33.70 AAAA ATOM 2850 N ARG À 356 15.591 46.610 68.065 1.00 33.70 AAAA ATOM 2852 CB ARG À 356 14.901 46.197 65.772 1.00 29.50 AAAA ATOM 2853 CG ARG À 356 15.635 47.423 65.255 1.00 33.70 AAAA ATOM 2853 CG ARG À 356 16.418 47.194 63.373 1.00 29.50 AAAA ATOM 2856 NP ARG À 356 17.955 48.455 63.371 1.00 29.50 AAAA ATOM 2856 CZ ARG À 356 11.914 61.97 65.772 1.00 29.50 AAAA ATOM 2858 NP ARG À 356 11.915 68.455 67.773 1.00 29.50 AAAA ATOM 2858 NP ARG À 356 11.915 68.455 67.773 1.00 29.50 AAAA ATOM 2860 C ARG À 356 11.916 48.00 ARG | | | aa 1 | א מימווו | 355 | 17.959 | 47.052 | 71.695 | 1.00 49.91 | AAAA |
|--|------|------|------|----------|-------|--------|---------|---------|--------------|--------|
| ATOM 2841 CE2 ARE A 355 19.684 45.888 72.627 1.00 52.03 AAAA ATOM 2842 CE3 TRP A 355 18.038 44.450 71.548 1.00 50.53 AAAA ATOM 2843 CE3 TRP A 355 18.886 47.915 72.284 1.00 50.53 AAAA ATOM 2844 CE3 TRP A 355 18.886 47.915 72.284 1.00 50.53 AAAA ATOM 2845 CE2 TRP A 355 20.060 44.763 73.003 1.00 52.64 AAAA ATOM 2846 CC3 TRP A 355 20.060 44.763 73.003 1.00 52.64 AAAA ATOM 2846 CC3 TRP A 355 20.060 44.763 73.003 1.00 52.64 AAAA ATOM 2846 CC3 TRP A 355 15.788 47.767 68.675 1.00 40.28 AAAA ATOM 2849 O TRP A 355 15.788 47.767 68.675 1.00 33.02 AAAAA ATOM 2849 O TRP A 355 15.788 47.767 68.675 1.00 33.02 AAAAA ATOM 2849 O TRP A 355 15.788 47.767 68.675 1.00 33.82 AAAAA ATOM 2851 CA ARG A 356 14.401 46.365 67.225 1.00 33.70 AAAA ATOM 2851 CA ARG A 356 14.901 46.397 65.772 1.00 29.50 AAAA ATOM 2851 CA ARG A 356 14.901 46.197 65.772 1.00 29.50 AAAA ATOM 2854 CD ARG A 356 15.635 47.423 65.256 1.00 25.22 AAAAA ATOM 2855 CC ARG A 356 17.976 48.533 62.574 1.00 17.06 AAAA ATOM 2855 CC ARG A 356 17.976 48.533 62.574 1.00 17.06 AAAA ATOM 2855 CC ARG A 356 17.976 48.533 62.574 1.00 17.06 AAAA ATOM 2856 CC ARG A 356 17.976 48.533 62.741 1.00 17.06 AAAA ATOM 2856 CC ARG A 356 18.403 47.451 61.919 1.00 17.66 AAAAA ATOM 2856 CC ARG A 356 18.403 47.451 61.919 1.00 17.66 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAA ATOM 2866 CC ARG A 356 18.445 49.721 62.241 1.00 17.66 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.33 AAAAA ATOM 2866 CC ARG A 356 13.605 44.117 67.011 1.00 34.47 AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA | MOTA | 2839 | | TRP A | 355 | | | | | AAAA |
| ATOM 2842 CES TRP A 355 | | | | | | | | | | AAAA |
| ATOM 2842 CLL 14FR A 355 18.846 47.915 72.284 1.00 50.53 AAAA ATOM 2844 NEI TER A 355 20.460 44.763 73.003 1.00 52.64 AAAA ATOM 2846 C.22 TER A 355 20.460 44.763 73.003 1.00 52.64 AAAA ATOM 2846 C.22 TER A 355 20.460 44.763 73.003 1.00 52.64 AAAA ATOM 2846 CLL TER A 355 20.008 43.518 72.642 1.00 53.02 AAAA ATOM 2849 C TER A 355 15.788 47.767 68.675 1.00 40.28 AAAA ATOM 2849 C TER A 355 15.788 47.767 68.675 1.00 33.62 AAAA ATOM 2849 C TER A 355 15.788 47.767 68.675 1.00 33.62 AAAA ATOM 2849 C TER A 356 15.591 46.610 68.065 1.00 33.62 AAAA ATOM 2850 N ARG A 356 14.440 46.365 67.225 1.00 33.70 AAAA ATOM 2851 CA ARG A 356 14.901 46.397 65.772 1.00 29.50 AAAA ATOM 2852 CB ARG A 356 15.635 47.423 65.256 1.00 25.22 AAAA ATOM 2854 CD ARG A 356 15.635 47.423 65.256 1.00 25.22 AAAA ATOM 2855 CZ ARG A 356 17.975 48.533 63.571 1.00 18.55 AAAA ATOM 2855 CZ ARG A 356 17.976 48.533 63.571 1.00 18.55 AAAA ATOM 2855 CZ ARG A 356 17.976 48.533 63.571 1.00 18.55 AAAA ATOM 2859 C ZARG A 356 18.403 47.451 61.919 1.00 17.66 AAAA ATOM 2859 C ZARG A 356 18.403 47.451 61.919 1.00 17.66 AAAA ATOM 2859 C ZARG A 356 13.605 44.117 67.051 1.00 34.63 AAAA ATOM 2850 N ZARG A 356 13.605 44.117 67.051 1.00 34.53 AAAA ATOM 2866 CZ ARG A 356 13.605 44.117 67.051 1.00 34.53 AAAA ATOM 2866 CZ ARG A 356 13.605 44.117 67.051 1.00 34.53 AAAA ATOM 2866 N GLY A 357 13.503 44.117 67.051 1.00 34.53 AAAA ATOM 2866 N GLY A 357 13.503 44.117 67.051 1.00 34.53 AAAA ATOM 2866 N GLY A 357 11.536 44.117 67.051 1.00 34.53 AAAA ATOM 2866 N GLY A 357 11.536 44.117 67.051 1.00 34.53 AAAA ATOM 2866 N GLY A 357 11.506 44.117 67.051 1.00 34.57 AAAA ATOM 2866 N GLY A 358 9.118 49.91 48.419 1.00 03.4.47 AAAA ATOM 2866 N GLY A 358 9.118 49.91 48.419 1.00 03.3.94 AAAA ATOM 2867 C GLY A 358 9.118 49.91 48.419 1.00 03.4.47 AAAA ATOM 2867 C GLY A 358 9.118 49.91 48.419 1.00 33.94 AAAA ATOM 2867 C GLY A 358 9.118 49.91 48.419 1.00 33.94 AAAA ATOM 2867 C GLY A 358 9.118 49.91 48.419 1.00 33.94 AAAA ATOM 2887 C GLY A 358 9.118 49.91 48.91 48.91 48.91 48.91 48.91 48.91 48.91 48.9 | | | | | | | | | 1.00 52.25 | AAAA |
| ATOM 2845 C22 TER A 355 | | | | | | | | | | AAAA |
| ARMA 2845 C22 TRP A 355 | | | | | | | | | | AAAA |
| ATOM 2846 C.23 TRP A 355 18.810 43.352 71.921 1.00 53.02 AAAA ATOM 2847 C.23 TRP A 355 15.017 48.520 68.675 1.00 40.28 AAAA ATOM 2848 C TRP A 355 15.017 48.720 68.675 1.00 40.28 AAAA ATOM 2849 C TRP A 355 15.017 48.720 68.675 1.00 39.82 AAAA ATOM 2850 N ARC 356 15.5017 48.720 68.691 1.00 39.82 AAAA ATOM 2850 N ARC 356 15.5017 48.720 68.591 1.00 33.70 33.70 AAAA ATOM 2851 CA ARG A 356 14.440 46.365 67.225 1.00 33.70 AAAA ATOM 2852 CB ARG A 356 14.440 46.365 67.225 1.00 29.50 AAAA ATOM 2852 CB ARG A 356 14.440 46.365 67.225 1.00 29.50 AAAA ATOM 2853 CB ARC A 356 15.613 4.901 46.197 65.772 1.00 29.50 AAAA ATOM 2854 CD ARC A 356 17.055 48.435 63.536 1.00 11.56 AAAA ATOM 2855 CD ARC A 356 17.055 48.435 63.533 1.00 18.55 AAAA ATOM 2855 CD ARC A 356 17.055 48.435 63.533 1.00 18.55 AAAA ATOM 2859 NIL ARC A 356 18.403 47.451 61.991 1.00 17.66 AAAA ATOM 2859 NIL ARC A 356 18.403 47.451 61.991 1.00 17.66 AAAA ATOM 2859 NIL ARC A 356 18.403 47.451 62.241 1.00 17.65 AAAA ATOM 2869 NIL ARC A 356 13.605 44.117 67.051 1.00 35.86 AAAA ATOM 2860 O ARC A 356 13.605 44.117 67.051 1.00 34.63 AAAA ATOM 2861 N GLY A 357 13.567 45.112 69.079 1.00 34.58 AAAA ATOM 2862 CA GLY A 357 13.567 45.112 69.079 1.00 34.58 AAAA ATOM 2865 N GLY A 357 13.567 45.112 69.079 1.00 34.58 AAAA ATOM 2865 N GLY A 357 11.536 47.8117 67.051 1.00 34.61 AAAA ATOM 2865 N GLY A 358 9.468 42.566 69.916 1.00 34.43 AAAA ATOM 2865 N GLY A 358 9.468 42.566 69.916 1.00 34.41 AAAA AAAA ATOM 2867 C GLY A 358 9.468 42.566 69.916 1.00 34.51 AAAA AAAA ATOM 2867 N GLY A 358 9.468 42.566 69.916 1.00 34.51 AAAA AAAA ATOM 2867 N GLY A 358 9.468 42.566 69.916 1.00 34.51 AAAAA AAAA ATOM 2867 N GLY A 358 9.468 42.566 69.916 1.00 34.51 AAAAA AAAA AAAA AAAA AAAA AAAA AAAA | | | | | | | | | 1.00 52.64 | AAAA |
| ATOM 2847 CH2 TRP A 355 | | • | | | | | | | 1.00 53.12 | AAAA |
| ATOM 2849 C TRP 3 355 15.788 47.767 68.675 1.00 40.28 AAAA ATOM 2849 O TRP 3 355 15.017 48.720 68.591 1.00 39.82 AAAA ATOM 2851 CA ARG A 356 15.591 46.610 68.065 1.00 36.83 AAAA ATOM 2851 CA ARG A 356 14.440 46.365 67.225 1.00 29.50 AAAA ATOM 2852 CB ARG A 356 14.440 46.365 67.225 1.00 29.50 AAAA ATOM 2853 CG ARG A 356 14.440 46.365 67.225 1.00 29.50 AAAA ATOM 2855 NE ARG A 356 17.056 48.450 47.423 63.572 1.00 29.50 AAAA ATOM 2855 NE ARG A 356 17.056 48.435 63.533 1.00 21.53 AAAA ATOM 2855 NE ARG A 356 17.056 48.435 63.533 1.00 18.55 AAAA ATOM 2858 NH2 ARG A 356 17.976 48.533 62.574 1.00 17.06 AAAA ATOM 2859 NH2 ARG A 356 18.403 47.451 61.991 1.00 17.64 AAAA ATOM 2859 NH2 ARG A 356 18.403 47.451 61.991 1.00 17.64 AAAA ATOM 2859 NH2 ARG A 356 13.631 45.005 67.7733 1.00 34.53 AAAA ATOM 2869 NH2 ARG A 356 13.631 45.005 67.7733 1.00 34.53 AAAA ATOM 2861 N GLY A 357 13.587 46.411 67.051 1.00 34.63 AAAA ATOM 2863 C C ARG A 356 13.601 44.117 67.051 1.00 34.63 AAAA ATOM 2863 C C GLY A 357 13.003 43.590 99.734 1.00 34.33 AAAA ATOM 2863 C C GLY A 357 13.003 43.590 99.734 1.00 34.58 AAAA ATOM 2866 C GLY A 357 13.003 43.590 99.734 1.00 34.58 AAAA ATOM 2866 C GLY A 357 11.006 44.418 69.935 1.00 34.58 AAAA ATOM 2867 C GLY A 357 11.006 44.418 69.935 1.00 34.51 AAAA ATOM 2867 C GLY A 358 10.876 42.006 70.139 1.00 34.51 AAAA ATOM 2867 C GLY A 358 10.876 42.006 70.139 1.00 34.51 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.468 42.556 69.936 1.00 34.61 AAAA ATOM 2868 C GLY A 359 9.508 89.908 1.00 34.61 AAAA ATOM 2869 N GLU A 359 9.508 89.908 1.00 34.61 AAAA ATOM 2869 N GLU A 359 9.508 89.908 1.00 34.61 AAAA ATOM 2869 C C GLY A 359 9.508 89.908 89.908 1.00 34.61 AAAA ATOM 2877 C GLU A 359 9.508 89.908 89. | | | | | | | | | 1.00 53.02 | AAAA |
| ATOM 2849 0 TRP A 3555 15.037 48.720 68.591 1.00 39.82 AAAA ATOM 2851 CA ARG A 356 15.591 46.610 68.065 1.00 36.83 AAAA ATOM 2851 CA ARG A 356 14.940 46.365 67.225 1.00 33.70 AAAA ATOM 2852 CB ARG A 356 14.940 46.365 67.225 1.00 29.50 AAAA ATOM 2853 CG ARG A 356 14.940 46.365 67.225 1.00 29.50 AAAA ATOM 2854 CD ARG A 356 14.940 46.396 67.225 1.00 29.50 AAAA ATOM 2855 NE ARG A 356 15.635 47.423 65.256 1.00 25.22 AAAA ATOM 2855 NE ARG A 356 16.418 47.194 63.973 1.00 17.06 AAAA ATOM 2856 CZ ARG A 356 17.055 48.435 63.533 1.00 18.55 AAAA ATOM 2857 NH1 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2858 NH2 ARG A 356 18.443 47.216 62.241 1.00 17.06 AAAA ATOM 2858 NH2 ARG A 356 18.443 49.721 62.241 1.00 17.64 AAAA ATOM 2858 NH2 ARG A 356 13.831 45.095 67.773 1.00 34.63 AAAA ATOM 2860 O ARG A 356 13.831 45.095 67.773 1.00 34.63 AAAA ATOM 2861 N GLY A 357 13.567 45.112 69.099 1.00 34.58 AAAA ATOM 2862 CA GLY A 357 13.567 45.112 69.099 1.00 34.58 AAAA ATOM 2862 O GLY A 357 11.536 43.783 69.395 1.00 34.33 AAAA ATOM 2866 CA GLY A 357 11.536 43.783 69.395 1.00 34.33 AAAA ATOM 2866 CA GLY A 357 11.536 47.2966 70.139 1.00 34.58 AAAA ATOM 2866 CA GLY A 358 9.468 42.566 69.916 1.00 34.61 AAAA ATOM 2866 CA GLY A 358 9.468 42.566 69.916 1.00 34.61 AAAA ATOM 2866 CA GLY A 358 9.468 42.566 69.916 1.00 34.61 AAAA ATOM 2866 CA GLY A 358 9.144 41.389 70.555 1.00 34.47 AAAA ATOM 2867 C GLY A 358 9.962 40.821 71.345 1.00 34.47 AAAA ATOM 2868 O GLY A 358 9.914 41.389 70.555 1.00 34.47 AAAA ATOM 2868 O GLY A 358 9.914 41.389 70.555 1.00 34.47 AAAA ATOM 2867 C GLU A 359 7.869 9.094 70.555 1.00 34.47 AAAA ATOM 2874 CBL GLU A 359 3.00 39.644 71.774 1.00 34.78 AAAA ATOM 2875 CBL GLU A 359 3.00 39.644 71.775 1.00 34.77 AAAA ATOM 2875 CBL GLU A 359 3.00 39.644 71.776 1.00 34.78 AAAA ATOM 2875 CBL GLU A 359 3.00 39.644 71.776 1.00 34.25 AAAAA ATOM 2877 CBL GLU A 359 3.00 39.644 71.776 1.00 34.25 AAAAA ATOM 2878 CBL GLU A 359 3.00 39.644 71.776 1.00 34.25 AAAAA ATOM 2879 CBL GLU A 359 3.00 39.644 71.776 1.00 34.20 AAAAA ATOM 2889 CC ARG A 3 | | | | | | | | | 1.00 40.28 | AAAA |
| ATOM 2850 N ARG A 356 ATOM 2851 CA ARG A 356 ATOM 2852 CB ARG A 356 ATOM 2852 CB ARG A 356 ATOM 2853 CG ARG A 356 ATOM 2853 CG ARG A 356 ATOM 2854 CD ARG A 356 ATOM 2855 NE ARG A 356 ATOM 2857 NH1 ARG A 356 ATOM 2857 NH1 ARG A 356 ATOM 2858 NH2 ARG A 356 ATOM 2859 CD ARG A 356 ATOM 2859 NH2 ARG A 356 ATOM 2859 NH2 ARG A 356 ATOM 2859 NH2 ARG A 356 ATOM 2869 NH2 ARG A 356 ATOM 2869 NH2 ARG A 356 ATOM 2861 N GUY A 357 ATOM 2861 N GUY A 357 ATOM 2863 CC GUY A 357 ATOM 2863 CC GUY A 357 ATOM 2863 CC GUY A 357 ATOM 2866 N GUY A 357 ATOM 2867 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2867 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2867 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2867 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2867 N GUY A 358 ATOM 2868 N GUY A 358 ATOM 2869 N GUY A 359 ATOM 2870 C GUY A 360 ATOM 2889 C C ARG A 361 AT | | | | | | | | | 1.00 39.82 | AAAA |
| ATOM 2851 CA ARG A 356 14.440 46.365 67.225 1.00 33.70 AAAA ATOM 2852 CB ARG A 356 14.901 46.197 65.772 1.00 29.50 AAAA ATOM 2853 CG ARG A 356 15.635 47.423 65.256 1.00 25.22 AAAA ATOM 2855 NE ARG A 356 15.635 47.423 65.256 1.00 25.22 AAAA ATOM 2855 NE ARG A 356 17.055 48.435 62.574 1.00 17.66 AAAA ATOM 2857 NH1 ARG A 356 17.976 48.435 62.574 1.00 17.66 AAAA ATOM 2857 NH1 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 C ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 C ARG A 356 13.811 45.095 62.241 1.00 17.64 AAAA ATOM 2859 C ARG A 356 13.811 45.095 67.051 1.00 34.63 AAAA ATOM 2850 C ARG A 356 13.811 45.095 67.073 1.00 34.63 AAAA ATOM 2860 O ARG A 356 13.811 45.095 67.051 1.00 34.43 AAAA ATOM 2860 C ARG A 357 11.536 44.117 67.051 1.00 34.58 AAAA ATOM 2860 C ARG A 357 11.536 43.783 69.395 1.00 34.31 AAAA ATOM 2864 O GLY A 357 11.536 43.783 69.395 1.00 34.31 AAAA ATOM 2866 CA GLY A 357 11.536 43.783 69.395 1.00 34.31 AAAA ATOM 2866 CA GLY A 358 10.876 42.996 70.139 1.00 34.67 AAAA ATOM 2866 CA GLY A 358 9.148 42.556 69.916 1.00 34.67 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.47 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.47 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.47 AAAA ATOM 2867 C G GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA ATOM 2867 C G GLY A 358 9.148 42.556 69.916 1.00 34.61 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.61 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.61 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.61 AAAA ATOM 2868 O GLY A 358 9.148 42.556 69.916 1.00 34.67 AAAA ATOM 2867 C GLY A 358 9.148 42.556 69.916 1.00 34.67 AAAA ATOM 2868 O GLY A 358 9.154 AAAA ATOM 2868 O GLY A 359 AAAAA ATOM 2868 O GLY A 359 AAAA ATOM 2868 O GLY A 359 | | | | | | | | | 1.00 36.83 | AAAA |
| ATOM 2851 CB ARG A 356 | | | | | | | | | 1.00 33.70 | AAAA |
| ATOM 2853 CG ARG A 356 | | | | | | | | | 1.00 29.50 | AAAA |
| ATOM 2854 CD ARG A 356 15.418 47.194 63.973 1.00 21.53 AAAA ATOM 2856 CZ ARG A 356 17.976 48.533 62.574 1.00 17.06 AAAAA ATOM 2857 NH1 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2858 NH2 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2858 NH2 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 C ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 C ARG A 356 13.631 45.095 67.773 1.00 34.63 AAAA ATOM 2850 C ARG A 356 13.605 44.117 67.051 1.00 35.86 AAAA ATOM 2861 N GLY A 357 13.003 43.96 59.734 1.00 34.58 AAAA ATOM 2862 CA GLY A 357 11.006 44.418 68.484 1.00 33.55 AAAA ATOM 2863 C GLY A 357 11.006 44.418 68.484 1.00 33.55 AAAA ATOM 2865 N GLY A 358 9.464 9.221 62.296 70.139 1.00 34.47 AAAA ATOM 2865 N GLY A 358 9.464 42.566 69.916 1.00 34.61 AAAA ATOM 2865 N GLY A 358 9.464 42.566 69.916 1.00 34.61 AAAA ATOM 2869 N GLY A 358 9.962 40.821 71.345 1.00 34.47 AAAA ATOM 2869 N GLU A 359 7.869 40.948 70.523 1.00 34.47 AAAA ATOM 2869 N GLU A 359 7.869 40.948 70.523 1.00 34.47 AAAA ATOM 2867 N GLU A 359 7.869 40.948 70.523 1.00 34.78 AAAA ATOM 2870 CA GLU A 359 7.869 40.948 70.523 1.00 34.78 AAAA ATOM 2870 CA GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2870 CA GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2870 CA GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 34.92 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 38.52 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2870 CA GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2880 CB GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2880 CB GLU A 360 AAAA ATOM | | | | | | | | | 1.00 25.22 | AAAA |
| ATOM 2855 NE ARG A 356 17.055 48.435 63.533 1.00 18.55 AAAA ATOM 2856 CZ ARG A 356 17.076 48.533 62.574 1.00 17.06 AAAA ATOM 2857 NH1 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2858 NH2 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 C ARG A 356 13.605 44.117 67.051 1.00 34.63 AAAA ATOM 2860 O ARG A 356 13.605 44.117 67.051 1.00 34.63 AAAA ATOM 2860 O ARG A 356 13.605 44.117 67.051 1.00 34.63 AAAA ATOM 2861 N GLY A 357 13.587 45.112 69.079 1.00 34.53 AAAA ATOM 2862 CA GLY A 357 13.587 45.112 69.079 1.00 34.53 AAAA ATOM 2863 C GLY A 357 11.536 43.783 69.395 1.00 34.53 AAAA ATOM 2865 N GLY A 357 11.536 43.783 69.395 1.00 34.63 AAAA ATOM 2865 C GLY A 357 11.066 44.418 68.484 1.00 33.56 AAAA ATOM 2865 C GLY A 358 10.876 42.906 70.139 1.00 34.67 AAAA ATOM 2865 C GLY A 358 10.876 42.906 70.139 1.00 34.67 AAAA ATOM 2865 C GLY A 358 9.146 42.656 69.916 1.00 34.67 AAAA ATOM 2867 C GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA ATOM 2867 C GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA ATOM 2867 C GLY A 358 9.144 41.89 70.655 1.00 34.61 AAAA ATOM 2869 N GLU A 359 7.869 40.981 71.345 1.00 34.27 AAAA ATOM 2869 N GLU A 359 7.869 40.982 71.180 1.00 34.61 AAAA ATOM 2870 CA GLU A 359 7.869 40.982 71.180 1.00 34.78 AAAA ATOM 2870 CA GLU A 359 7.869 40.982 71.180 1.00 34.78 AAAA ATOM 2870 CA GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2877 CB GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2877 CB GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2877 CB GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2877 CB GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2877 CB GLU A 359 3.910 44 71.174 1.00 34.78 AAAA ATOM 2878 C GLU A 359 3.017 40.108 71.600 1.00 39.65 AAAAA ATOM 2878 C GLU A 359 3.058 42.234 71.584 1.00 38.29 AAAA ATOM 2878 C GLU A 359 3.017 40.108 71.600 1.00 32.63 AAAA ATOM 2880 C GLU A 359 3.058 44.600 71.918 71.750 1.00 32.90 AAAA ATOM 2881 C GLU A 359 3.058 68.600 67.02 57.000 91.00 32.00 AAAA ATOM 2880 C GLU A 350 600 91.000 91.000 91.000 91.000 91.000 91.000 91.000 91.000 91.000 91.0 | | | | | | | | | | AAAA |
| ATOM 2855 CZ ARG A 356 17.976 48.533 62.574 1.00 17.06 AAAA ATOM 2857 NH1 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 NH2 ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 CZ ARG A 356 18.403 47.451 61.919 1.00 17.64 AAAA ATOM 2859 CZ ARG A 356 18.405 49.721 62.241 1.00 11.56 AAAA ATOM 2860 N GLY A 357 13.003 43.96 69.7374 1.00 34.63 AAAA ATOM 2861 N GLY A 357 13.003 43.96 69.7374 1.00 34.58 AAAA ATOM 2862 CA GLY A 357 11.006 44.418 68.484 1.00 33.55 AAAA ATOM 2863 C GLY A 357 11.006 44.418 68.484 1.00 33.55 AAAA ATOM 2865 CA GLY A 358 9.468 42.906 70.139 1.00 34.47 AAAA ATOM 2866 CA GLY A 358 9.468 42.656 69.916 1.00 34.47 AAAA ATOM 2868 N GLY A 358 9.468 42.656 69.916 1.00 34.47 AAAA ATOM 2868 N GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA ATOM 2868 N GLY A 358 9.124 41.389 70.655 1.00 34.47 AAAA ATOM 2868 N GLY A 358 9.124 41.389 70.655 1.00 34.47 AAAA ATOM 2867 C GLY A 358 9.124 41.389 70.655 1.00 34.47 AAAA ATOM 2868 N GLY A 358 9.124 41.389 70.655 1.00 34.47 AAAA ATOM 2867 C GLY A 358 9.124 41.389 70.655 1.00 34.47 AAAA ATOM 2870 CA GLU A 359 7.438 39.729 71.180 1.00 33.94 AAAA ATOM 2870 CA GLU A 359 5.210 39.644 71.174 1.00 34.78 AAAA ATOM 2871 CB GLU A 359 5.210 39.644 71.174 1.00 34.78 AAAA ATOM 2873 C GLU A 359 5.278 40.648 72.123 1.00 36.70 AAAA ATOM 2873 C GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2873 C GLU A 359 3.863 41.020 71.740 1.00 38.52 AAAAA ATOM 2875 C GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2875 C GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2876 C GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2877 C GLU A 359 3.863 41.020 71.740 1.00 32.92 AAAA ATOM 2878 N VAL A 360 7.339 37.35 71.036 1.00 32.29 AAAA ATOM 2878 N VAL A 360 7.339 37.35 71.036 1.00 32.29 AAAA ATOM 2880 C VAL A 360 7.339 37.35 71.036 1.00 32.99 AAAA ATOM 2880 C VAL A 360 7.339 35.319 69.976 1.00 32.99 AAAA ATOM 2881 C C ARG A 361 7.084 36.56 68.674 1.00 33.99 AAAA ATOM 2880 C C ARG A 361 7.086 36.608 62.978 1.00 33.12 AAAA ATOM 2889 C C ARG A 361 7.086 36.608 62.978 1.00 33 | | | | | | | | | 1.00 18.55 | AAAA |
| ATOM 2857 NH1 ARG A 356 | | | | | | | | | 1.00 17.06 | AAAA |
| ATOM 2859 NHL ARG A 356 18.445 49.721 62.241 1.00 11.56 AAAA ATOM 2859 C ARG A 356 13.831 45.095 67.773 1.00 34.63 AAAA ATOM 2860 N GLY A 357 13.003 43.960 69.734 1.00 34.58 AAAA ATOM 2861 N GLY A 357 13.003 43.960 69.734 1.00 34.33 AAAA ATOM 2863 C GLY A 357 11.536 43.783 69.395 1.00 34.31 AAAA ATOM 2864 O GLY A 357 11.006 44.418 68.484 1.00 33.55 AAAA ATOM 2865 N GLY A 357 11.006 44.418 68.484 1.00 34.33 AAAA ATOM 2866 C GLY A 358 9.468 42.906 70.139 1.00 34.47 AAAA ATOM 2866 N GLY A 358 9.468 42.906 70.139 1.00 34.47 AAAA ATOM 2866 C GLY A 358 9.468 42.656 69.916 1.00 34.61 AAAA ATOM 2866 O GLY A 358 9.468 42.656 69.916 1.00 34.47 AAAA ATOM 2867 C GLY A 358 9.428 40.948 70.523 1.00 34.47 AAAA ATOM 2868 N GLU A 359 7.869 40.948 70.523 1.00 34.17 AAAA ATOM 2868 N GLU A 359 7.483 39.729 71.180 1.00 33.94 AAAA ATOM 2870 CA GLU A 359 5.278 40.648 7.2.123 1.00 36.70 AAAA ATOM 2870 CG GLU A 359 5.278 40.648 72.123 1.00 36.70 AAAA ATOM 2870 CG GLU A 359 5.278 40.648 72.123 1.00 36.70 AAAA ATOM 2870 CG GLU A 359 3.007 40.108 71.600 1.00 38.40 AAAA ATOM 2870 CG GLU A 359 3.007 40.108 71.600 1.00 38.55 AAAA ATOM 2873 CD GLU A 359 3.007 40.108 71.600 1.00 38.55 AAAA ATOM 2873 CD GLU A 359 3.007 40.108 71.600 1.00 38.55 AAAA ATOM 2875 CG GLU A 359 3.007 40.108 71.600 1.00 38.55 AAAA ATOM 2875 CG GLU A 359 3.007 40.108 71.600 1.00 38.52 AAAA ATOM 2875 CG GLU A 359 3.007 40.108 71.600 1.00 38.52 AAAA ATOM 2875 CC GLU A 359 3.007 40.108 71.600 1.00 38.52 AAAA ATOM 2878 N AAA AAA AAA AAA AAA AAA AAAA AAAA | | | CZ | ARG A | 356 | | | | 1.00 17.64 | AAAA |
| ATOM 2859 C ARG A 356 13.605 44.117 67.051 1.00 34.63 AAAA AROM 2860 O ARG A 356 13.605 44.117 67.051 1.00 34.58 AAAA AROM 2861 N GLY A 357 13.003 43.960 69.734 1.00 34.58 AAAA AROM 2862 CA GLY A 357 13.003 43.960 69.734 1.00 34.31 AAAA AROM 2863 C GLY A 357 11.006 44.418 68.484 1.00 33.56 AAAA AROM 2866 CA GLY A 357 11.006 44.418 68.484 1.00 33.56 AAAA AROM 2866 CA GLY A 358 9.110 0.07 1.00 34.47 AAAA AROM 2866 CA GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA AROM 2866 CA GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA AROM 2869 N GLY A 358 9.962 40.821 71.345 1.00 34.47 AAAA AROM 2869 N GLY A 358 9.962 40.821 71.345 1.00 34.16 AAAA AROM 2871 CB GLY A 359 7.869 40.948 70.523 1.00 34.16 AAAA AROM 2871 CB GLY A 359 5.910 39.644 71.174 1.00 33.94 AAAA AROM 2871 CB GLY A 359 5.910 39.644 71.174 1.00 34.78 AAAA AROM 2872 CG GLY A 359 5.910 39.644 71.174 1.00 34.78 AAAA AROM 2873 CD GLU A 359 5.910 39.644 71.174 1.00 36.70 AAAA AROM 2873 CD GLU A 359 5.910 39.644 71.174 1.00 36.70 AAAA AROM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 39.55 AAAA AROM 2875 CEZ GLU A 359 8.658 38.549 70.648 72.123 1.00 39.55 AAAA AROM 2875 CEZ GLU A 359 8.058 38.549 70.640 1.00 39.55 AAAA AROM 2875 CEZ GLU A 359 8.058 38.549 70.464 1.00 39.55 AAAA AROM 2876 C GLU A 359 8.058 38.549 70.464 1.00 32.26 AAAA AROM 2878 C GLU A 359 8.058 38.549 70.464 1.00 32.26 AAAA AROM 2880 CB VAL A 360 9.422 35.472 71.376 1.00 32.92 AAAA AROM 2881 CGI VAL A 360 9.422 35.472 71.376 1.00 32.92 AAAA AROM 2881 CGI VAL A 360 9.422 35.472 71.376 1.00 32.99 AAAA AROM 2881 CGI VAL A 360 10.521 36.406 70.791 1.00 32.99 AAAA AROM 2882 CB ARG A 361 6.046 71.827 71.00 32.99 AAAA AROM 2882 CB ARG A 361 6.066 33.577 64.99 1.00 33.52 AAAA AROM 2889 CD ARG A 361 6.035 34.508 66.086 1.00 33.52 AAAA AROM 2889 CD ARG A 361 6.066 33.057 68.557 1.00 32.99 AAAA AROM 2889 CD ARG A 361 6.066 33.057 68.557 1.00 34.18 AAAA AROM 2889 CD ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA AROM 2889 CD ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA AROM 2899 CD ARG A 361 6.066 33.057 68.557 1 | | | | | | | | | 1.00 11.56 | AAAA |
| ATOM 2859 C ARG A 356 ATOM 2860 O ARG A 356 ATOM 2861 N GLY A 357 ATOM 2861 N GLY A 357 ATOM 2862 CA GLY A 357 ATOM 2863 C GLY A 357 ATOM 2863 C GLY A 357 ATOM 2865 N GLY A 357 ATOM 2865 N GLY A 357 ATOM 2865 N GLY A 357 ATOM 2866 CA GLY A 358 ATOM 2867 C GLY A 358 ATOM 2867 C GLY A 358 ATOM 2868 O GLY A 358 ATOM 2869 N GLU A 359 ATOM 2870 CA GLU A 359 ATOM 2871 CB GLU A 359 ATOM 2871 CB GLU A 359 ATOM 2873 CD GLU A 359 ATOM 2873 CD GLU A 359 ATOM 2873 CD GLU A 359 ATOM 2874 CB GLU A 359 ATOM 2875 CB GLU A 359 ATOM 2876 CB GLU A 359 ATOM 2877 CB GLU A 359 ATOM 2878 CB GLU A 359 ATOM 2879 CB GLU A 359 ATOM 2880 CB VAL A 360 ATOM 2880 CB ARG A 361 ATOM 2880 CB ARG A 361 ATOM 2880 CB | | | | | | | | | | AAAA |
| ATOM 2861 N GLY A 357 13.003 43.96 69.734 1.00 34.58 AAAA ATOM 2862 CA GLY A 357 13.003 43.96 69.734 1.00 34.33 AAAA ATOM 2863 C GLY A 357 11.006 44.418 68.484 1.00 33.56 AAAA ATOM 2865 N GLY A 358 9.468 42.656 69.916 1.00 34.47 AAAA ATOM 2866 CA GLY A 358 9.468 42.656 69.916 1.00 34.47 AAAA ATOM 2866 CA GLY A 358 9.468 42.656 69.916 1.00 34.47 AAAA ATOM 2866 N GLY A 358 9.962 40.821 71.345 1.00 34.47 AAAA ATOM 2866 N GLY A 358 9.962 40.821 71.345 1.00 34.47 AAAA ATOM 2866 N GLY A 358 9.962 40.821 71.345 1.00 34.47 AAAA ATOM 2870 CA GLU A 359 7.489 40.948 70.523 1.00 34.16 AAAA ATOM 2871 CB GLU A 359 7.499 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2871 CB GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2872 CG GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 39.95 AAAA ATOM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 39.95 AAAA ATOM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 39.95 AAAA ATOM 2873 CD GLU A 359 3.598 42.234 71.584 1.00 32.286 AAAA ATOM 2875 OE2 GLU A 359 3.598 42.234 71.584 1.00 32.286 AAAA ATOM 2878 N VAL A 360 7.918 37.375 71.036 1.00 32.26 AAAA ATOM 2878 N VAL A 360 7.918 37.375 71.036 1.00 32.26 AAAA ATOM 2880 CB VAL A 360 9.422 35.472 71.375 1.00 32.92 AAAA ATOM 2881 CG VAL A 360 10.521 36.406 71.827 1.00 32.29 AAAA ATOM 2881 CG VAL A 360 10.521 36.406 71.827 1.00 32.99 AAAA ATOM 2881 CG VAL A 360 10.521 36.406 70.791 1.00 32.99 AAAA ATOM 2884 O VAL A 360 10.521 36.406 71.827 1.00 32.99 AAAA ATOM 2885 C AARG A 361 6.035 34.508 68.086 1.00 33.43 AAAA ATOM 2889 C AARG A 361 6.035 34.508 62.978 1.00 31.70 AAAA ATOM 2889 C ARG A 361 6.035 34.508 68.086 1.00 33.79 AAAA ATOM 2889 C ARG A 361 6.036 34.508 62.978 1.00 31.70 AAAA ATOM 2889 C ARG A 361 6.036 34.508 62.978 1.00 31.70 AAAA ATOM 2889 C ARG A 361 6.036 34.508 62.978 1.00 31.70 AAAA ATOM 2889 C ARG A 361 6.036 34.508 62.978 1.00 31.70 AAAA ATOM 2889 C ARG A 361 6.036 63.31 64.96 61.901 1.00 31.70 AAAA ATOM 2889 C ARG A 361 6.036 63.305 68.508 60.996 1.00 31.70 AAAA ATOM 2899 C ARG A 361 6.066 30 | | | | ARG A | 356 | | | | 1.00 35.86 | AAAA |
| ATOM 2861 N GLY A 357 13.003 43.960 59.734 1.00 34.33 AAAA ATOM 2863 C GLY A 357 11.536 43.783 69.395 1.00 34.31 AAAA ATOM 2865 N GLY A 358 10.876 42.906 70.139 1.00 34.47 AAAA ATOM 2866 CA GLY A 358 9.468 42.656 69.916 1.00 34.61 AAAA ATOM 2866 CA GLY A 358 9.468 42.656 69.916 1.00 34.61 AAAA ATOM 2867 C GLY A 358 9.114 41.389 70.655 1.00 34.47 AAAA ATOM 2869 N GLU A 359 7.869 40.948 70.523 1.00 34.61 AAAA ATOM 2869 N GLU A 359 7.869 40.948 70.523 1.00 34.16 AAAA ATOM 2871 CB GLU A 359 7.438 39.729 71.180 1.00 34.78 AAAA ATOM 2872 CG GLU A 359 5.910 39.644 71.174 1.00 34.78 AAAA ATOM 2873 CD GLU A 359 5.278 40.648 72.123 1.00 34.61 AAAA ATOM 2873 CD GLU A 359 3.017 40.108 71.600 1.00 39.65 AAAA ATOM 2873 CD GLU A 359 3.017 40.108 71.600 1.00 39.65 AAAA ATOM 2875 OE2 GLU A 359 3.017 40.108 71.600 1.00 39.65 AAAA ATOM 2877 C GLU A 359 8.058 38.549 70.464 1.00 32.86 AAAA ATOM 2877 O GLU A 359 8.058 38.549 70.464 1.00 32.86 AAAA ATOM 2879 C GLU A 359 8.058 38.549 70.464 1.00 32.92 AAAA ATOM 2879 C GLU A 359 8.078 8.058 38.549 70.464 1.00 32.92 AAAA ATOM 2879 CA VAL A 360 7.918 37.375 71.036 1.00 32.92 AAAA ATOM 2879 CA VAL A 360 7.918 37.375 71.036 1.00 32.99 AAAA ATOM 2880 CB VAL A 360 9.422 35.477 71.376 1.00 32.99 AAAA ATOM 2881 CG1 VAL A 360 10.017 34.252 70.701 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.093 35.319 69.976 1.00 32.99 AAAA ATOM 2883 C VAL A 360 6.702 34.660 70.791 1.00 32.09 AAAA ATOM 2883 C VAL A 360 6.702 34.660 70.791 1.00 32.09 AAAA ATOM 2885 C AARG A 361 6.046 7.339 35.319 69.976 1.00 33.12 AAAA ATOM 2889 CB ARG A 361 6.046 7.893 36.526 6.555 1.00 33.43 AAAA ATOM 2889 CB ARG A 361 6.046 7.938 36.526 6.555 1.00 33.43 AAAA ATOM 2889 CB ARG A 361 6.046 7.938 36.526 6.555 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 6.046 7.938 36.526 6.555 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 6.046 7.339 35.319 69.976 1.00 32.02 AAAA ATOM 2889 CD ARG A 361 6.046 7.084 35.527 68.968 1.00 33.79 AAAA ATOM 2899 CC ARG A 361 6.046 7.039 36.550 68.968 1.00 33.79 AAAA ATOM 2899 C C ARG A 361 6.066 33.057 68.955 1.00 33.79 A | | | | | | | | | 1.00 34.58 | AAAA |
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| ATOM 2873 CD GLU A 359 3.863 41.020 71.740 1.00 38.40 AAAA ATOM 2874 OEI GLU A 359 3.017 40.108 71.600 1.00 39.65 AAAA ATOM 2875 OE2 GLU A 359 8.058 38.549 70.464 1.00 32.86 AAAA ATOM 2877 O GLU A 359 8.678 38.692 69.427 1.00 32.92 AAAA ATOM 2877 O GLU A 359 8.678 38.692 69.427 1.00 32.92 AAAA ATOM 2878 N VAL A 360 7.918 37.375 71.036 1.00 32.63 AAAA ATOM 2879 CA VAL A 360 8.480 36.215 70.409 1.00 32.70 AAAA ATOM 2880 CE VAL A 360 9.422 35.472 71.375 1.00 32.29 AAAA ATOM 2881 CGI VAL A 360 10.017 34.252 70.701 1.00 32.99 AAAA ATOM 2882 CG2 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.02 AAAA ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2888 CG ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2888 CG ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.99 AAAA ATOM 2889 CD ARG A 361 7.084 35.321 68.674 1.00 33.90 AAAA ATOM 2889 CD ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2889 CD ARG A 361 7.084 35.321 68.076 1.00 34.35 AAAA ATOM 2899 NE ARG A 361 7.084 35.321 68.076 1.00 34.35 AAAA ATOM 2899 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAAA ATOM 2899 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAAA ATOM 2899 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAAA ATOM 2899 CC ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2899 CC ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CC ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CC ARG A 361 7.068 36.562 61.941 1.00 31.70 AAAAA ATOM 2899 CC ARG A 361 7.084 31.226 69.756 1.00 34.09 AAAA ATOM 2899 CC ARG A 361 7.084 31.226 69.918 1.00 31.70 AAAAA ATOM 2899 CC ARG A 361 7.084 31.226 69.968 1.00 33.79 AAAA ATOM 2899 CC ARG A 361 7.086 31.00 30.552 AAAA ATOM 2899 CC ARG A 361 7.086 31.00 30.552 AAAA ATOM 2899 CC ARG A 361 7.086 31.00 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CC ARG A 361 7.086 31.00 30.555 68.401 1.00 31.408 AAAA ATOM 2899 CC ARG A 361 7.086 31.00 30.555 68. | | | | | | | | 72.123 | | |
| ATOM 2873 OE2 GLU A 359 3.017 40.108 71.600 1.00 39.65 AAAA ATOM 2875 OE2 GLU A 359 8.588 8.549 70.464 1.00 32.86 AAAA ATOM 2877 O GLU A 359 8.678 38.692 69.427 1.00 32.92 AAAA ATOM 2877 O GLU A 359 8.678 38.692 69.427 1.00 32.92 AAAA ATOM 2878 N VAL A 360 7.918 37.375 71.036 1.00 32.63 AAAA ATOM 2887 CA VAL A 360 9.422 35.472 71.376 1.00 32.99 AAAA ATOM 2880 CB VAL A 360 10.017 34.252 70.701 1.00 32.99 AAAA ATOM 2881 CG1 VAL A 360 10.521 36.406 71.827 1.00 32.99 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.09 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.430 36.552 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 7.086 36.562 61.941 1.00 31.70 AAAA ATOM 2893 NH2 ARG A 361 7.080 36.608 62.978 1.00 31.70 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 33.79 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 33.79 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 37.80 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 37.80 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 37.80 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 37.80 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 37.80 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 37.80 AAAA ATOM 2899 CD ARG A 361 7.068 36.552 61.941 1.00 39.85 AAAA ATOM 2890 CD ARG A 361 7.068 36.552 61.9 | | | | | | | | 71.740 | | |
| ATOM 2876 C GLU A 359 8.058 38.549 70.464 1.00 32.86 AAAA ATOM 2877 O GLU A 359 8.678 38.692 69.427 1.00 32.92 AAAA ATOM 2878 N VAL A 360 8.480 36.215 70.409 1.00 32.70 AAAA ATOM 2879 CA VAL A 360 9.422 35.472 71.376 1.00 32.99 AAAA ATOM 2880 CB VAL A 360 10.017 34.252 70.701 1.00 32.99 AAAA ATOM 2881 CG1 VAL A 360 10.521 36.406 71.827 1.00 32.99 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.09 AAAA ATOM 2883 C VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2885 CB ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.041 35.972 64.469 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2889 CD ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2891 CZ ARG A 361 7.068 36.552 61.941 1.00 33.90 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.552 61.941 1.00 33.90 AAAA ATOM 2893 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2895 C ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2895 C ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2895 C ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2895 C ARG A 361 7.430 36.355 66.855 1.00 33.90 AAAA ATOM 2895 C ARG A 361 7.430 36.552 61.941 1.00 30.48 AAAA ATOM 2895 C ARG A 361 7.430 36.552 61.941 1.00 30.48 AAAA ATOM 2895 C ARG A 361 7.430 36.552 61.941 1.00 30.48 AAAA ATOM 2895 C ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2895 C ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.70 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.70 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.70 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.70 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.80 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.80 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.80 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.80 AAAA ATOM 2895 C ARG A 361 7.068 36.555 68.782 1.00 37.80 AAAA A | | | OFI | | | | 40.108 | 71.600 | | |
| ATOM 2876 C GLU A 359 8.058 38.549 70.464 1.00 32.86 AAAA ATOM 2877 O GLU A 359 8.678 38.692 69.427 1.00 32.92 AAAA ATOM 2878 N VAL A 360 7.918 37.375 71.036 1.00 32.63 AAAA ATOM 2879 CA VAL A 360 8.480 36.215 70.409 1.00 32.70 AAAA ATOM 2880 CB VAL A 360 10.017 34.252 70.701 1.00 32.99 AAAA ATOM 2881 CG1 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2882 CG2 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.81 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2885 N ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.035 34.508 66.565 1.00 33.43 AAAA ATOM 2888 CG ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2889 CD ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2890 NE ARG A 361 7.430 36.502 64.469 1.00 33.90 AAAA ATOM 2891 CZ ARG A 361 7.430 36.502 61.941 1.00 30.48 AAAA ATOM 2899 NE ARG A 361 7.430 36.502 61.941 1.00 30.48 AAAA ATOM 2899 NH2 ARG A 361 7.430 36.502 61.941 1.00 30.48 AAAA ATOM 2899 NH2 ARG A 361 7.430 36.502 61.941 1.00 30.48 AAAA ATOM 2899 CR ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2899 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CR ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2899 CR ARG A 361 7.890 36.502 61.941 1.00 30.48 AAAA ATOM 2899 CR ARG A 361 7.890 36.502 61.941 1.00 30.48 AAAA ATOM 2899 CR ARG A 361 7.890 36.502 61.941 1.00 30.48 AAAA ATOM 2899 CR ARG A 361 7.068 36.552 61.941 1.00 30.48 AAAA ATOM 2899 CR ARG A 361 7.01 32.537 68.968 1.00 33.79 AAAA ATOM 2899 CR LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CR LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CR LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2903 C LYS A 362 2.208 33.446 68.420 1.00 35.12 AAAA ATOM 2903 C LYS A 362 2.208 33.446 68.42 | | | | GIJI A | 359 | | 42.234 | 71.584 | | |
| ATOM 2877 N VAL A 360 7.918 37.375 71.036 1.00 32.63 AAAA ATOM 2879 CA VAL A 360 9.422 35.472 71.376 1.00 32.70 AAAA ATOM 2881 CGI VAL A 360 10.017 34.252 70.701 1.00 32.99 AAAA ATOM 2882 CG2 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.09 AAAA ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2885 CG ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2886 CA ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2887 CB ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2891 CZ ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2892 NH1 ARG A 361 7.084 36.331 64.193 1.00 31.70 AAAA ATOM 2893 NH2 ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.086 36.562 61.941 1.00 30.48 AAAA ATOM 2899 CD ARG A 361 7.006 36.948 62.802 1.00 29.71 AAAA ATOM 2899 CD ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2899 CD LYS A 362 4.914 32.407 68.991 1.00 35.62 AAAA ATOM 2899 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2899 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 34.14 | | | | GLU A | 359 | | | 70.464 | | |
| ATOM 2878 N VAL A 360 | | | | | | 8.678 | 38.692 | 69.427 | | |
| ATOM 2880 CB VAL A 360 9.422 35.472 71.376 1.00 32.70 AAAA ATOM 2881 CG1 VAL A 360 10.017 34.252 70.701 1.00 32.99 AAAA ATOM 2882 CG2 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.81 AAAA ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2886 CG ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2888 CG ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2893 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2894 C ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2895 O ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2895 O ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2895 CD ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2895 CD ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2895 O ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2895 CD ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2896 CD LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2896 CD LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2897 CA LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2890 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2901 CC LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2901 CC LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2901 CC LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2901 CC LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2901 CC LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CC LYS A 362 2.473 34.909 68.45 | | | | | | 7.918 | 37.375 | | | |
| ATOM 2880 CB VAL A 360 9.422 35.472 70.701 1.00 32.99 AAAA ATOM 2881 CG1 VAL A 360 10.017 34.252 70.701 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.81 AAAA ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2888 CG ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2893 NH2 ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2894 C ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2895 O ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2897 CA ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2897 CA ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2897 CA LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.487 1.00 34.14 | | | | | | 8.480 | 36.215 | | | |
| ATOM 2881 CG1 VAL A 360 10.017 34.252 70.701 1.00 32.09 AAAA ATOM 2882 CG2 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.81 AAAA ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2887 CB ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 5.731 35.885 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2893 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2894 C ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2895 N ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2895 C ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 34.14 | | | | | | 9.422 | 35.472 | | | |
| ATOM 2882 CG2 VAL A 360 10.521 36.406 71.827 1.00 32.09 AAAA ATOM 2883 C VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2894 C ARG A 361 9.162 36.948 62.802 1.00 32.971 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 35.62 AAAAA ATOM 2900 CD LYS A 362 2.378 31.446 68.420 1.00 37.80 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 35.12 AAAA ATOM 2900 CD LYS A 362 2.908 33.446 68.420 1.00 35.12 AAAA ATOM 2900 CD LYS A 362 2.908 33.446 68.420 1.00 35.12 AAAA ATOM 2900 CD LYS A 362 2.908 33.446 68.420 1.00 35.12 AAAA ATOM 2900 CD LYS A 362 2.908 33.446 68.420 1.00 35.12 AAAA ATOM 2900 CD LYS A 362 2.908 33.446 68. | | | CG1 | | | 10.017 | | | | |
| ATOM 2883 C VAL A 360 7.339 35.319 69.976 1.00 32.02 AAAA ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2893 NH2 ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2897 CA LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2897 CA LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2890 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2901 CE LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 2.473 34.909 68.451 1.00 3 | | | | | | 10.521 | | 71.827 | | |
| ATOM 2884 O VAL A 360 6.702 34.660 70.791 1.00 32.02 AAAA ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2894 C ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 | | | | | | 7.339 | 35.319 | | | |
| ATOM 2885 N ARG A 361 7.084 35.321 68.674 1.00 33.12 AAAA ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.52 AAAA ATOM 2887 CB ARG A 361 6.148 34.558 66.565 1.00 33.43 AAAA ATOM 2888 CG ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.430 36.331 64.193 1.00 31.18 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.808 31.022 68.961 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 69.777 1.00 42.09 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 34.14 | | | | | | 6.702 | 34.660 | | | |
| ATOM 2886 CA ARG A 361 6.035 34.508 68.086 1.00 33.32 AAAA ATOM 2887 CB ARG A 361 5.731 35.885 66.565 1.00 33.43 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.808 31.022 68.968 1.00 33.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2898 CB LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.208 33.4909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 | | | | | | 7.084 | | | 1.00 33.12 | |
| ATOM 2887 CB ARG A 361 6.148 34.558 65.565 1.00 34.35 AAAA ATOM 2888 CG ARG A 361 5.731 35.885 65.967 1.00 34.35 AAAA ATOM 2889 CD ARG A 361 6.041 35.972 64.469 1.00 31.70 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2891 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2895 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 34.14 | | | | | | 6.035 | | | | |
| ATOM 2888 CG ARG A 361 5.731 35.885 65.967 1.00 33.90 AAAA ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.70 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2894 C ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2895 O ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 N LYS A 362 4.914 32.407 68.496 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA AAAA AAAA AAAA AAAA AAAA AAAA | | | | ARG A | A 361 | 6.148 | | • | | |
| ATOM 2889 CD ARG A 361 | | | _ | ARG A | A 361 | | | | | |
| ATOM 2890 NE ARG A 361 7.430 36.331 64.193 1.00 31.18 AAAA ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 31.18 AAAA ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2899 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | | | | 6.041 | 35.972 | 64.469 | | |
| ATOM 2891 CZ ARG A 361 7.890 36.608 62.978 1.00 30.48 AAAA ATOM 2892 NH1 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 34.20 AAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2898 CB LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | | ARG I | A 361 | 7.430 | | | 1.00 31.70 | |
| ATOM 2892 NH1 ARG A 361 7.068 36.562 61.941 1.00 30.48 AAAA ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 29.71 AAAA ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2898 CB LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 NZ LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | | ARG A | A 361 | 7.890 | | | 1.00 31.16 | |
| ATOM 2893 NH2 ARG A 361 9.162 36.948 62.802 1.00 34.20 AAAA ATOM 2894 C ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 34.68 AAAA ATOM 2896 N LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2898 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | | L ARG | A 361 | | 36.562 | | 1.00 30.48 | |
| ATOM 2894 C ARG A 361 6.066 33.057 68.557 1.00 34.20 AAAA ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2897 CA LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2898 CB LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 C LYS A 362 5.710 30.177 68.005 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA AAAA | | | | 2 ARG | A 361 | 9.162 | | | 1.00 29.71 | |
| ATOM 2895 O ARG A 361 7.101 32.537 68.968 1.00 33.79 AAAA ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.68 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | - | | | ARG A | A 361 | 6.066 | | | 1.00 34.20 | |
| ATOM 2896 N LYS A 362 4.914 32.407 68.496 1.00 34.08 AAAA ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.62 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2902 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | _ | _ | ARG | A 361 | 7.101 | | | 1.00 33.79 | |
| ATOM 2897 CA LYS A 362 4.808 31.022 68.901 1.00 35.02 AAAA ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2904 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2904 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | _ | LYS | A 362 | | | | | |
| ATOM 2898 CB LYS A 362 3.350 30.555 68.782 1.00 37.80 AAAA ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 40.38 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | | LYS . | A 362 | | | | | |
| ATOM 2599 CG LYS A 362 2.378 31.226 69.756 1.00 42.09 AAAA ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | | | LYS | A 362 | | 30.555 | 68.782 | | |
| ATOM 2900 CD LYS A 362 2.505 32.777 69.777 1.00 42.09 AAAA ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 34.14 AAAA | | - | | | | | | | | |
| ATOM 2901 CE LYS A 362 2.208 33.446 68.420 1.00 41.94 AAAA AAAA 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 6.425 29.301 68.487 1.00 34.14 AAAA | | | | LYS | A 362 | | | | | |
| ATOM 2902 NZ LYS A 362 2.473 34.909 68.451 1.00 39.85 AAAA ATOM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATOM 2903 C LYS A 362 6.425 29.301 68.487 1.00 34.14 AAAA | | | | LYS | A 362 | | | | | |
| ATCM 2903 C LYS A 362 5.710 30.177 68.005 1.00 35.12 AAAA ATCM 2903 C LYS A 362 6.425 29.301 68.487 1.00 34.14 AAAA | | | | LYS | A 362 | | | | | |
| AAAA | | | | | | | | | | |
| VION PA | | | | | | 6.42 | 5 29.30 | 1 68.48 | 7 1.00 34.14 | , whun |
| | AIOM | | • | • | - | | | | | |

| • | | | | | | | | | |
|--------|-------|-----|------------|------|----------|--------|--------|--------------|-------|
| MOTA | 2905 | Ν. | GLU | A 36 | 3 5.661 | 30.460 | 66.703 | 1.00 35.12 | AAAA |
| | | | GLU | | | 29.741 | 65.699 | 1.00 35.62 | |
| MOTA | 2906 | CA | | | | | | | AAAA |
| ATOM | 2907 | CB | GLU | A 36 | 3 6.567 | 30.560 | 64.424 | 1.00 36.81 | AAAA |
| ATOM | 2908 | CG | GLU | A 36 | 3 5.280 | 30.808 | 63.711 | 1.00 38.66 | AAAA |
| ATOM | 2909 | CD | GLU | | | 31.704 | 62.517 | 1.00 39.60 | AAAA |
| | | | | | | | | | |
| ATOM - | 2910 | | GLU | | | 31.324 | 61.637 | 1.00 39.11 | AAAA |
| ATOM | 2911 | OE2 | GLU | A 36 | 3 4.826 | 32.782 | 62.469 | 1.00 39.95 | AAAA |
| ATOM | 2912 | C · | GLU | A 36 | 3 7.836 | 29.450 | 66.181 | 1.00 35.14 | ÄAAA |
| | | | | | | | | 1.00 34.50 | |
| AŢOM | 2913 | 0 | GLU | | | 28.316 | 66.098 | | AAAA |
| MOTA | 2914 | N | Δ L | A 36 | 4 8.475 | 30.505 | 66.671 | 1.00 34.96 | AAAA |
| MOTA | 2915 | CA | VAL | A 36 | 4 9.830 | 30.431 | 67.180 | 1.00 34.44 | AAAA |
| | 2916 | CB | VAL | | | 31.821 | 67.570 | 1.00 33.68 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2917 | | VAL | | | 31.722 | | - 1.00 34.13 | AAAA |
| MOTA | 2918 | CG2 | VAL | A 36 | 4 10.337 | 32.715 | 66.347 | 1.00 31.83 | AAAA |
| ATOM | 2919 | С | VAL | A 36 | 4 9.908 | 29.499 | 68.370 | 1.00 34.44 | AAAA |
| | | | VAL | | | 28.640 | | | |
| MOTA | 2920 | 0 | | | | | 68.430 | 1.00 36.01 | -AAAA |
| ATOM | 2921 | N | LYS | A 36 | 5 8.980 | 29.649 | 69.305 | 1.00 33.27 | AAAA |
| MOTA | 2922 | CA | LYS | A 36 | 5 8.970 | 28.790 | 70.476 | 1.00 33.20 | AAAA |
| | 2923 | CB | LYS | | | 29.319 | 71.508 | 1.00 34.28 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2924 | CG | LYS | | | 30.705 | 72.033 | 1.00 33.67 | AAAA |
| ATOM | 2925 | CD | LYS | A 36 | 5 7.282 | 31.181 | 73.039 | 1.00 34.85 | AAAA |
| ATOM | 2926 | CE | LYS | A 36 | 5 7.658 | 32.534 | 73.638 | 1.00 36.47 | AAAA |
| | 2927 | NZ | LYS | | | 32.990 | 74.710 | 1.00 37.91 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2928 | С | LYS | | | 27.342 | 70.109 | 1.00 32.75 | AAAA |
| MOTA | 2929 | 0 | LYS | A 36 | 5 9.071 | 26.421 | 70.818 | 1.00 31.95 | AAAA |
| ATOM | 2930 | N | ASP | A 36 | 6 7.919 | 27.136 | 69.012 | 1.00 32.81 | AAAA |
| ATOM | 2931 | CA | ASP | | | 25.777 | 68.581 | 1.00 33.65 | AAAA |
| | | | | | | | | | |
| MOTA | 2932 | CB | ASP | | | 25.726 | 67.557 | 1.00 33.98 | AAAA |
| MOTA | 2933 | CG | ASP | A 36 | 6 5.131 | 26.107 | 68.140 | 1.00 33.94 | AAAA |
| ATOM | 2934 | OD1 | ASP | A 36 | 6 4.870 | 25.767 | 69.307 | 1.00 33.89 | AAAA |
| ATOM | 2935 | 002 | ASP | A 36 | 6 4.332 | 26.722 | 67.412 | 1.00 35.08 | AAAA |
| | 2936 | c | ASP | | | 25.167 | 67.940 | 1.00 33.05 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2937 | 0 | ASP | | | 24.006 | 68.172 | 1.00 33.66 | AAAA |
| MOTA | 2938 | N | THR | A 36 | 7 9.473 | 25.959 | 67.102 | 1.00 33.07 | AAAA |
| MOTA | 2939 | CA | THR | A 36 | 7 10.684 | 25.540 | 66.412 | 1.00 32.27 | AAAA |
| ATOM | 2940 | CB | THR | | | 26.719 | 65.641 | 1.00 32.28 | AAAA |
| | | | | | | 27.039 | 64.520 | 1.00 30.64 | AAAA |
| ATOM | 2941 | OG1 | THR | | | | | | |
| MOTA | 2942 | CG2 | THR | | | 26.377 | 65.166 | 1.00 33.29 | AAAA |
| MOTA | 2943 | С | THR | A 36 | 7 11.680 | 25.044 | 67.442 | 1.00 31.71 | AAAA |
| ATOM | 2944 | 0 | THR | A 36 | 7 12.178 | 23.918 | 67.352 | 1.00 30.45 | AAAA |
| | 2945 | N | LEU | | | 25.896 | 68.426 | 1.00 32.05 | AAAA |
| ATOM | | | | | | | | | |
| ATOM | 2946 | CA | LEU | | | 25.560 | 69.482 | 1.00 32.49 | AAAA |
| ATOM | 2947 | CB | LEU | A 36 | 8 13.085 | 26.749 | 70.421 | 1.00 32.27 | AAAA |
| ATOM | 2948 | CG | LEU | A 36 | 8 14.097 | 27.809 | 69.960 | 1.00 32.71 | AAAA |
| ATOM | 2949 | | LEU | | | 27.170 | 69.899 | 1.00 33.00 | AAAA |
| | | | | | | 28 393 | 68.597 | 1.00 31.86 | AAAA |
| MOTA | 2950 | | LEU | | | | | | |
| ATOM | 2951 | С | LEU | A 36 | 8 12.455 | 24.334 | 70.256 | 1.00 33.82 | AAAA |
| ATOM | 2952 | 0 | LEU | A 36 | B 13.266 | 23.133 | 70.489 | 1.00 34.29 | AAAA |
| ATOM | 2953 | N | GLU | A 36 | 9 11.183 | 24.285 | 70.645 | 1.00 34.30 | AAAA |
| | 2954 | CA | GLU | | | 23.135 | 71.375 | 1.00 36.07 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2955 | CB | GLU | | | 23.319 | 71.748 | 1.00 38.71 | AAAA |
| ATOM | 2956 | CG | GLU | A 36 | 9 8.974 | 24.285 | 72.920 | 1.00 40.18 | AAAA |
| ATOM | 2957 | CD | GLU | A 36 | 7.509 | 24.359 | 73.341 | 1.00 41.56 | AAAA |
| | .2958 | | GLU . | | | 23.276 | 73.572 | 1.00 41.83 | AAAA |
| | | | | | | | | | |
| ATOM | 2959 | | GLU | | | 25.489 | 73.451 | 1.00 41.74 | AAAA |
| ATOM | 2960 | С | GLU | A 36 | 9 10.893 | 21.822 | 70.611 | 1.00 37.16 | AAAA |
| ATOM | 2961 | 0 | GLU | A 36 | 9 11.338 | 20.831 | 71.196 | 1.00 37.00 | AAAA |
| | 2962 | N | LYS | | | 21.788 | 69.315 | 1.00 37.71 | AAAA |
| ATOM | | | | | | | | | |
| MOTA | 2963 | CA | LYS . | | | 20.547 | 68.567 | 1.00 38.46 | AAAA |
| MOTA | 2964 | CB | LYS . | a 37 | 0 10.166 | 20.604 | 67.177 | 1.00 39.96 | AAAA |
| ATOM | 2965 | CG | LYS . | | | 20.532 | 67.186 | 1.00 42.68 | AAAA |
| ATOM | 2966 | CD | LYS | | | 20.320 | 65.775 | 1.00 44.54 | AAAA |
| | | | | | | | | 1.00 45.55 | AAAA |
| atom | 2967 | CE | LYS . | | | 20.075 | 65.781 | | |
| MOTA | 2968 | NZ | LYS | A 37 | 6.009 | 19.797 | 64.409 | 1.00 45.50 | AAAA |
| MOTA | 2969 | С | LYS . | A 37 | 12.282 | 20.235 | 68.452 | 1.00 38.34 | AAAA |
| ATOM | 2970 | Ö | LYS | A 37 | 12.683 | 19.071 | 68.493 | 1.00 37.86 | AAAA |
| ALUM. | 25.0 | - | | | | | | | |

| ATOM | 2971 | N | ALA | Α | 371 | 13.1 | 05 | 21.266 | 68.311 | - | 37.69 | AAAA |
|------------------|--------|----------|------------|--------|--------|--------------|-----|------------------|------------------|------|----------------|--------------|
| MOTA | 2972 | | ALA | | | 14.5 | 43 | 21.057 | 68.226 | _ | 37.20 | AAAA |
| ATOM | 2973 | CB | ALA | Α | 371 | 15.2 | 58 | 22.375 | 67.936 | | 35.48 | AAAA |
| ATOM | 2974 | C | ALA | Α | 371 | 15.0 | | 20.477 | 69.558 | | 37.63 | AAAA |
| ATOM | 2975 | 0 | ALA | Α | 371 | 15.9 | | 19.626 | 69.585 | | 37.12 | AAAA |
| MOTA | 2976 | | LYS | | | 14.4 | | 20.930 | 70.665 | | 37.59 | AAAA |
| ATOM | 2977 | CA | LYS | А | 372 | 14.7 | | | .71.995 | | 37.46 | AAAA |
| MOTA | 2978 | CB | LYS | A | 372 | 14.0 | | 21.156 | 73.095 | | 36.52 | AAAA |
| MOTA | 2979 | CG | LYS | A | 372 | 14.2 | | 22.634 | 73.111 | | 22.67 | AAAA |
| MOTA | 2980 | CD | LYS | A | 372 | 13.3 | | 23.396 | 74.022 | | 22.67 | AAAA |
| MOTA | 2981 | CE | LYS | | | 13.6 | | 24.874 | 73.901 | | 22.67 | AAAA |
| ATOM | 2982 | NZ | LYS | | _ | 12.6 | | 25.708 | 74.785 | | 22.67 | AAAA |
| MOTA | 2983 | С | LYS | Α | 372 | 14.4 | | 18.957 | 72.077 | | 37.60 | AAAA |
| MOTA | 2984 | 0 | | | 372 | 15.3 | | 18.171 | 72.407 | | 37.26 | AAAA |
| MOTA | 2985 | N | ALA | | | 13.2 | | 18.595 | 71.789 | | 38.17 39.55 | AAAA AAAA |
| MOTA | 2986 | CA | ALA | | | 12.8 | | 17.206 | 71.829 | | | AAAA |
| MOTA | 2987 | CB | | | 373 | 11.3 | | 17.109 | 71.395 | | 39.34 41.02 | AAAA |
| MOTA | 2988 | C | | | 373 | 13.6 | | 16.277 | 70.972 71.561 | | 42.26 | AAAA |
| MOTA | 2989 | 0 | | | 373 | 14.3 | | 15.410 | 69.725 | | 42.06 | AAAA |
| MOTA | 2990 | | ALA | | | 13.6 | | 16.416 | 54.072 | | 27.38 | ZONE |
| HETATM | 2991 | ZN | ZN | | 951 | 23.6 | | 34.788 | 53.458 | | 31.95 | SAHA |
| HETATM | | 01 | SHA | | 1 | 24.5 | | 33.295 35:218 | 51.444 | | 33.51 | SAHA |
| HETATM | | 02 | SHA | | 1 | 24.2 24.5 | | 33.085 | 52.069 | | 34.03 | SAHA |
| HETATM | | NI | SHA | | 1 1 | 24.0 | | 34.053 | 51.246 | | 34.25 | SAHA |
| HETATM | | C1 | SHA | | 1 | 23.0 | | 33.625 | 50.259 | | 36.87 | SAHA. |
| HETATM | 2996 | C2 | SHA | | 1 | 23.5 | | 33.781 | 48.816 | | 39.33 | SAHA |
| HETATM | | C3 C4 | SHA | | ī | 22.4 | | 33.274 | 47.852 | | 40.86 | SAHA |
| HETATM HETATM | | .C5 | SHA | | ī | 21.5 | | 34.413 | 47.455 | | 43.37 | SAHA |
| HETATM | | C6 | SHA | | ī | 21.0 | | 34.017 | 46.092 | 1.00 | 46.72 | SAHA |
| HETATM | | C7 | SHA | | ī | 19.7 | | 34.714 | 45.787 | 1.00 | 48.75 | Saha |
| HETATM | 3002 | C8 | SHA | | ī | 19.9 | | 35.720 | 44.693 | 1.00 | 50.75 | SAHA |
| HETATM | 3003 | 03 | SHA | | 1 | 20.3 | | 35.467 | 43.575 | 1.00 | 51.08 | SAHA |
| HETATM | | N2 | SHA | | 1 | 19.5 | 91 | 36.956 | 45.085 | | 52.52 | SAHA |
| HETATM | | C9 | SHA | | 1 | 19.8 | 342 | 38.330 | 44.507 | | 54.25 | SAHA |
| HETATM | 3006 | | SHA | C | 1 | 19.3 | 243 | 39.431 | 45.215 | | 55.76 | SAHA |
| HETATM | 3007 | C11 | SHA | C | 1 | 19.4 | 123 | 40.804 | 44.727 | | 56.53 | SAHA |
| HETATM | | C12 | SHA | C | 1 | 20.3 | | 41.085 | 43.545 | | 56.58 | AHA |
| HETATM | | C13 | SHA | , C | | 20. | | 39.942 | 42.827 | | 55.93 | SAHA |
| HETATM | | C14 | SHA | C | | 20. | | 38.546 | 43.304 | | 54.65 | SAHA SOLV |
| HETATM | 3011 | | WAT | | | 36. | | 44.023 | 49.378 | 1.00 | | SOLV |
| HETATM | 3012 | | PAW | | | 27. | | 16.865 | 62.162 | 1.00 | 0 4.67 | SOLV |
| HETATM | | OH2 | | | | 23. | | 30.387 | 59.575 46.926 | | 0 21.13 | SOLV |
| HETATM | | | raw. | | | 33. | | 41.862 | 47.867 | | 23.72 | SOLV |
| HETATM | | | FAW | | | 24. | | 20.442 | 33.590 | | 0 18.19 | SOLV |
| H. TATM | 3016 | | LAW | | | 34. | 921 | 29.753 | 62.099 | | 0 20.79 | SOLV |
| H_TATM | 3017 | | VAT | | | 17. | | 6.978 | 64.018 | | 0 28.94 | SOLV |
| HL FATM | 3018 | | raw Paw | | | 35. | _ | 44.610 | 74.823 | | 0 31.62 | SOLV |
| HETATM | 3019 | | raw raw | | | 49. | | 27.797 | 65.303 | | 0 14.70 | SOLV |
| HETATM | 3020 | | LAW | | | 20. | | 34.049 | 61.067 | | 0 25.01 | SOLV |
| HETATM | 3021 | | LAW LAW | | | 44. | | 33.106 | 46.084 | 1.0 | 0 25.90 | SOLV |
| HETATM | 2022 | | LAW LAW | | | 22. | | 60.823 | 57.444 | 1.0 | 0 15.21 | SOLV |
| HETATM | 2023 | | WAT | | _ | | 399 | 32.742 | 65.163 | 1.0 | 0 20.66 | SOLV |
| HETATM HETATM | 2025 | | VA. | | | 32. | | 51.414 | 45.610 | 1.0 | 0 22.37 | SOLV |
| HETATM | 3025 | | WAT | | | 26. | | 42.873 | 73.427 | 1.0 | 0 27.86 | SOLV |
| HETATM | 3020 | | WAT | | | | 249 | 24.121 | 56.778 | | 0 15.09 | SOLV |
| HETAT | 3027 | | WAT | | | | 249 | 44.552 | 72.082 | | 0 40.95 | SOLV |
| HETAT | 3029 | | WAT | | | 26. | | 9.269 | 52.633 | | 0 26.66 | SOLV |
| HETAT | 1 3023 | | WA? | | | 26. | | 18.383 | 59.650 | | 0 11.42 | SOLV |
| HETATI | 1 3031 | OH2 | WA | ָרָ דָ | 22 | 39 | | 25.964 | 72.316 | | 0 20.32 | SOLV |
| HETATI | 1 3032 | | WAS | | | 26. | | 37.600 | 38.359 | | 0 37.22 | SOLV |
| HETATI | 1 3033 | | WAS | | | | 666 | 23.818 | 39.068 | | 0 32.27 | SOLV |
| HETAT | 1 3034 | OH2 | WA' | rī | 25 | | 714 | 52.213 | 70.663 | | 0 29.24 | SOLV |
| HETATI | 1 3035 | OH2 | WA' | r | 26 | 45. | 129 | 18.856 | 69.864 | | 0 29.58 | SOLV |
| HEADYA | 1 3036 | OH2 | WA' | r 1 | 27 | 30. | 024 | 17.886 | 49.758 | 1.0 | 0 15.52 | SOLV |
| HEIAII | | | | | | | | | - | | | • |

| HETATM | 3037 | OHO | WAT | n | 28 | 20.659 | 28.788 | 43.520 | 1.00 28.55 | cor |
|--------|------|-----|-----|---|-----|----------------|------------------|--------|------------|--------|
| HETATM | | | | | | | | | | SOLV |
| | | | WAT | | 29 | | 38.000 | 53.512 | 1.00 47.72 | SOLV |
| HETATM | | | TAW | | 30 | 18.285 | 29.333 | 54.536 | 1.00 21.34 | SOLV |
| HETATM | | | WAT | | 31 | 49.978 | 38.669 | 73.461 | 1.00 31.02 | SOLV |
| HETATM | | | WAT | | 32 | 21.587 | 50.386 | 71.043 | 1.00 14.52 | SOLV |
| HETATM | 3042 | OH2 | WAT | D | 33 | 46.784 | 32.121 | 33.375 | 1.00 31.79 | SOLV |
| HETATM | 3043 | OH2 | WAT | D | 34 | 33.359 | 39.755 | 49.117 | 1.00 16.13 | SOLV |
| HETATM | 3044 | OH2 | WAT | D | 35 | 7.687 | 37.657 | 51.568 | 1.00 27.22 | SOLV |
| HETATM | | OF2 | WAT | מ | 36 | 44.238 | 35.392 | 33.961 | 1.00 19.67 | SOLV |
| HETATM | | | WAT | | 37 | 10.908 | 25.384 | 58.206 | 1.00 33.51 | |
| HETATM | | | WAT | | 38 | 36.758 | 27.243 | 70.552 | | SOLV |
| HETATM | | | WAT | | 39 | | | | 1.00 39.61 | SOLV. |
| | _ | | WAT | | | 45.825 | 46.691 | 54.654 | 1.00 32.43 | SOLV |
| HETATM | | | | | 40 | 52.489 | 20.282 | 52.165 | 1.00 39.37 | SOLV |
| HETATM | | | WAT | | 42 | 12.117 | 17.831 | 56.596 | 1.00 27.74 | SOLV |
| HETATM | | | WAT | | 43 | 45.023 | 26.168 | 35.172 | 1.00 14.09 | SOLV |
| HETATM | | | WAT | _ | 44 | 39.392 | 12.771 | 62.066 | 1.00 35.15 | SOLV |
| HETATM | 3053 | OH2 | WAT | D | 45 | 3.930 | 26.970 | 63.814 | 1.00 22.23 | SOLV |
| HETATM | 3054 | OH2 | TAW | D | 46 | 8.454 | 19.321 | 71.677 | 1.00 32.36 | SOLV |
| HETATM | 3055 | QH2 | WAT | D | 47 | 20.280 | 18.126 | 73.237 | 1.00 33.88 | SOLV |
| HETATM | 3056 | OH2 | TAW | D | 48 | 9.321 | 39.409 | 54.873 | 1.00 18.57 | SOLV |
| HETATM | 3057 | OH2 | WAT | D | 49 | 50.852 | 41.323 | 58.048 | 1.00 21.25 | SOLV |
| HETATM | 3058 | OH2 | WAT | D | 50 | 37.134 | 34.599 | 60.315 | 1.00 61.70 | SOLV |
| HETATM | | OH2 | WAT | D | 51 | 14.944 | 62.815 | 48.613 | 1.00 42.50 | SOLV |
| HETATM | | | WAT | | 52 | 6.494 | 33.164 | 51.420 | 1.00 40.65 | SOLV |
| HETATM | | | WAT | | 53 | 24.913 | 44.799 | 72,298 | 1.00 17.10 | SOLV |
| HETATM | | | WAT | | 54 | 51.156 | 35.095 | 48.814 | 1.00 23.05 | |
| HETATM | | | WAT | | 55 | 16.518 | 41.750 | 45.596 | 1.00 49.25 | SOLV |
| HETATM | | | WAT | | 56 | 10.326 | | 61.267 | | SOLV |
| HETATM | | | WAT | | 57 | 25.316 | 16.413 47.708 | | 1.00 46.03 | SOLV |
| HETATM | | | WAT | | | | | 73.062 | 1.00 22.73 | SOLV |
| | | | | | 58 | 4.013 | 33.865 | 76.173 | 1.00 44.82 | SOLV |
| HETATM | | | WAT | | 59 | 24.846 | 18.072 | | 1.00 34.67 | SOLV |
| HETATM | | | WAT | | 60 | 15.930 | 56.853 | 61.737 | 1.00 55.56 | SOLV |
| HETATM | | | WAT | | 61 | 49.662 | 44.249 | 48.982 | 1.00 28.72 | SOLV |
| HETATM | | | TAW | | 62. | 23.232 | 17.421 | 53.920 | 1.00 13.11 | SOLV |
| HETATM | | | TAW | | 63 | 39.293 | 23.035 | 33.289 | 1.00 35.79 | SOLV |
| HETATM | | | WAT | | 64 | 19.908 | 20.169 | 44.339 | 1.00 24.33 | SOLV |
| HETATM | | | WAT | | 65 | 33.259 | 21.655 | 69.560 | 1.00 45.10 | SOLV |
| HETATM | | | WAT | | 66 | 27.528 | 53.947 | 68.629 | 1.00 44.79 | SOLV |
| HETATM | 3075 | OH2 | WAT | D | 67 | 18.774 | 48.716 | 52.865 | 1.00 54.01 | SOLV |
| METATM | 3076 | OH2 | TAW | D | 68 | 10.877 | 29.062 | 63.401 | 1.00 27.08 | SOLV |
| HETATM | 3077 | OH2 | TAW | D | 69 | 43.057 | 31.367 | 28.786 | 1.00 30.16 | SOLV |
| HETATM | 3078 | OH2 | WAT | D | 70 | 24.816 | 44.057 | 43.447 | 1.00 20.11 | SOLV |
| HETATM | 3079 | OH2 | TAW | D | 71 | 37.368 | 38.823 | 46.381 | 1.00 33.55 | SOLV |
| HETATM | 3080 | OH2 | WAT | D | 72 | 9.038 | 18.327 | 63.519 | 1.00 31.34 | SOLV |
| HETATM | | OH2 | WAT | D | 73 | 51.799 | 20.829 | 65,265 | 1.00 28.32 | · SOLV |
| HETATM | | | WAT | | 74 | 17.556 | 58.515 | 57.254 | 1.00 19.27 | SOLV |
| HETATM | | OH2 | WAT | D | 75 | 28.436 | 27.904 | 79.425 | 1.00 27.13 | SOLV |
| HETATM | | | WAT | _ | 76 | 18.939 | 35.798 | 35.800 | 1.00 94.18 | SOLV |
| HETATM | | | WAT | | 77 | 34.359 | 31.251 | 46.688 | 1.00 73.70 | SOLV |
| HETATM | | | WAT | | 78 | 44.373 | 51.649 | 60.029 | 1.00 30.23 | SOLV |
| HETATM | | | WAT | | 79 | 28.537 | 63.478 | 48.324 | 1.00 30.23 | |
| | | | | - | 80 | 6.869 | | | | SOLV |
| HETATM | | | WAT | | | | 44.113 | 72.030 | 1.00 28.59 | SOLV |
| HETATM | | | WAT | | 81 | 42.882 | 18.761 | 71.115 | 1.00 31.80 | SOLV |
| HETATM | | | TAW | | 82 | 36.712 | 59.078 | 53.901 | 1.00 40.11 | SOLV |
| HETATM | | | TAW | | 83 | 37.506 | 42.495 | 40.104 | 1.00 51.37 | SOLV |
| HETATM | | | TAW | | 84 | 40.054 | 38.439 | 55.415 | 1.00 20.07 | SOLV |
| HETATM | | | WAT | | 85 | 32.170 | 56.633 | 72.920 | 1.00 45.23 | SOLV |
| MTATEH | | | TAW | | 86 | 24.470 | 53.877 | 47.119 | 1.00 41.18 | SOLV |
| HETATM | 3095 | | TAW | | 87 | 48.585 | 35.663 | 67.518 | 1.00 33.40 | SOLV |
| MTATEK | 3096 | OH2 | WAT | Ð | 88 | 29.541 | 57.166 | 42.788 | 1.00 44.61 | SOLV |
| HETATM | 3097 | | TAW | | 89 | 47.814 | 28.707 | 41.228 | 1.00 45.64 | SOLV |
| HETATM | 3098 | OH2 | WAT | D | 90 | 49.377 | 52.112 | 63.320 | 1.00 22.26 | SOLV |
| HETATM | | OH2 | TAW | D | 91 | 44.219 | 43.589 | 43.912 | 1.00 39.90 | SOLV |
| HETATM | | OH2 | WAT | D | 92 | 25.913 | 61.639 | 75.382 | 1.00 48.28 | SOLV |
| HETATM | | | WAT | | 93 | 8.623 | 30.749 | 49.707 | 1.00 40.37 | SOLV |
| HETATM | | | WAT | | 94 | 45.634 | 41.080 | 40.990 | 1.00 21.46 | SOLV |
| | | | | - | _ | - - | | • | | |

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| HETATM | 3103 | OH2 | TAW | D | 95 | | 29.984 | 34.886 | 51.725 | 1.00 35.75 | SOLV |
|--------|------|-----|-----|---|-----|---|--------|--------|---------|--------------------------|------|
| HETATM | 3104 | OH2 | WAT | D | 96 | | 13.051 | 21.934 | 49.804 | 1.00 46.73 | SOLV |
| HETATM | | OH2 | TAW | D | 97 | | 32.412 | 65.913 | 55.822 | 1.00 43.39 | SOLV |
| HETATM | | OH2 | WAT | D | 98 | | 35.056 | 43.390 | 38.348 | 1.00 34.53 | SOLV |
| HETATM | | OH2 | WAT | D | 99 | | 22.360 | 47.680 | 60.688 | 1.00 19.16 | SOLV |
| HETATM | | OH2 | TAW | D | 100 | | 50.755 | 19.722 | 57.906 | 1.00 42.45 | SOLV |
| HETATM | | | WAT | | | | 7.875 | 37.690 | 74.094 | 1.00 37.18 | SOLV |
| HETATM | | | | | 102 | | 24.080 | 26.796 | 43.617 | 1.00 30.72 | SOLV |
| HETATM | | | WAT | | | | 45.206 | 34.126 | 75.765 | 1.00 39.89 | |
| HETATM | | _ | WAT | | | | 26.110 | 54.786 | 40.685 | 1.00 29.58 | |
| HETATM | | | WAT | | | | 25.918 | 39.658 | 77.647 | 1.00 44.04 | |
| | | | WAT | | | - | 41.578 | 18.191 | 36.809 | 1.00 42.22 | |
| HETATM | | | WAT | | | | 31.945 | 51.420 | 73.896 | 1.00 41.15 | |
| HETATM | | | WAT | | | | 16.722 | 60.311 | 51.182 | 1.00 48.74 | |
| HETATM | | | WAT | | | | 43.604 | 38.573 | 78.141 | 1.00 36.22 | |
| HETATM | | | | | | | 16.063 | 15.496 | 69.430 | 1.00 55.36 | |
| HETATM | | | WAT | | | | | 22.785 | 49.145 | 1.00 36.52 | |
| HETATM | | | WAT | | | | 21.630 | 56.647 | 44.026 | 1.00 50.82 | |
| HETATM | | | TAW | | | | 27.479 | | 61.674 | 1.00 35.55 | |
| HETATM | | | TAW | | | | 14.739 | 51.674 | 54.358 | | |
| HETATM | | | TAW | | | | 50.063 | 26.435 | | 1.00 50.86 1.00 44.21 | |
| HETATM | | | WAT | | | | 43.935 | 38.427 | 73.129 | | |
| HETATM | | | WAT | | | | 49.707 | 31.478 | 57.709 | 1.00 36.11 | |
| HETATM | | | WAT | | | | 25.032 | 43.463 | 55.676 | 1.00 38.06 | |
| HETATM | | | TAW | | | | 10.618 | 46.623 | 59.838 | 1.00 26.33 | |
| HETATM | 3127 | | TAW | | | | 48.466 | 33.382 | 61.437 | 1.00 19.82 | |
| HETATM | | | TAW | | | | 44.157 | 40.058 | .37.907 | 1.00 42.95 | · |
| HETATM | | | WAT | | | | 51.267 | 29.446 | 52.889 | 1.00 38.93 | |
| HETATM | 3130 | | WAT | | | | 16.653 | 15.228 | 72.975 | 1.00 45.41 | |
| HETATM | 3131 | | TAW | | | | 36.898 | 45.148 | 41.936 | 1.00 27.00 | |
| HETATM | 3132 | | WAT | | | | 49.655 | 34.591 | 59.117 | 1.00 38.97 | |
| HETATM | 3133 | | WAŢ | | | | 12.285 | 57.594 | 42.107 | 1.00 23.56 | |
| HETATM | 3134 | | WAT | | | | 28.294 | 57.644 | 73.289 | 1.00 34.79 | |
| HETATM | 3135 | | WAT | | | | 19.138 | 60.403 | 61.551 | 1.00 28.58 | |
| HETATM | 3136 | | WAT | | | | 30.300 | 33.685 | 34.047 | 1.00 27.37 | |
| HETATM | | | WAT | | | | 40.898 | 53.983 | 47.254 | 1.00 16.30 | |
| HETATM | 3138 | | WAT | | | | 43.550 | 32.160 | 38.272 | 1.00 38.86 | |
| HETATM | 3139 | | TAW | | | | 18.624 | 13.959 | 56.194 | 1.00 37.70 | |
| HETATM | | OH2 | WAT | D | 132 | | 18.580 | 12.901 | 62.894 | 1.00 27.28 | |
| HETATM | | OH2 | WAT | D | 133 | | 35.830 | 30.296 | 50.621 | 1.00 42.47 | |
| HETATM | | OH2 | WAT | D | 134 | | 51.219 | 35.855 | 51.878 | 1.00 20.37 | |
| HETATM | | OH2 | TAW | ם | 135 | | 50.428 | 22.486 | 49.267 | 1.00 39.37 | |
| HETATM | | OH2 | WAT | D | 136 | | 51.633 | 29.369 | 63.918 | 1.00 33.99 | |
| HETATM | | OH2 | WAT | D | 137 | | 46.384 | 43.924 | 55.825 | 1.00 22.63 | |
| HETATM | | OH2 | WAT | D | 138 | | 30.356 | 25.767 | 28.762 | 1.00 25.84 | |
| HETATM | | | TAW | | | | 25.070 | 47.842 | 60.819 | 1.00 25.00 | |
| HETATM | | OH2 | WAT | D | 140 | | 47.097 | 49.394 | 69.367 | 1.00 30.58 | |
| HETATM | | | WAT | | | | 15.246 | 37.581 | 73.398 | 1.00 36.82 | |
| HETATM | | | WAT | | | | 8.341 | 23.099 | 64.695 | 1.00 35.89 | |
| HETATM | | | WAT | | | | 30.065 | 18.220 | 46.048 | 1.00 14.26 | SOLV |
| HETATM | | OH2 | WAT | D | 144 | | 11.930 | 46.453 | 57.606 | 1.00 36.15 | SOLV |
| TELLEN | 22-2 | | | | | | | | | | |

INTERNATIONAL SEARCH REPORT

International application No. PCT/US00/24700

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|--|--|--|-------------------------|--|--|--|--|--|
| A. CLASSIFICATION OF SUBJECT MATTER | | | | | | | | |
| IPC(7) | :C07K 14/00; G01N 33/573 | | | | | | | |
| | US CL: Please See Extra Sheet. According to International Patent Classification (IPC) or to both national classification and IPC | | | | | | | |
| • | LDS SEARCHED | | | | | | | |
| | documentation searched (classification system follow | ed by classification sym | hole) | | | | | |
| | Please See Extra Sheet. | ed by classification sym | bois; | | | | | |
| 0.5. | t lease See Extra Sheet. | | | | | | | |
| Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched | | | | | | | | |
| Floatennia data harranta di Ariani | | | | | | | | |
| Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Extra Sheet. | | | | | | | | |
| C. DOCUMENTS CONSIDERED TO BE RELEVANT | | | | | | | | |
| Category* | Citation of document, with indication, where a | ppropriate, of the releva | unt passages | Relevant to claim No. | | | | |
| Y | KAKUTA et al. Crystal Structure of the Sulfotransferase Domain of Human Heparan Sulfate N-Deacetylase/N-Sulfotransferase 1. The Journal of Biological Chemistry. 16 April 1999, Volume 274, Number 16, pages 10673-10676, see especially the abstract. | | | | | | | |
| Y | SUEYOSHI et al. A role of Lys-614 in the sulfotransferase activity of human heparan sulfate N-deacetulase/N-sulfotransferase. FEBS Letters. 1998, Volume 433, pages 211-214, see especially the abstract. | | | | | | | |
| X Furth | ner documents are listed in the continuation of Box | C 🔲 s | G. J. | | | | | |
| | | | | | | | | |
| "A" doc | cial categories of cited documents: nument defining the general state of the art which is not considered so of particular relevance | date and not in | | mational filing date or priority ication but cited to understand invention | | | | |
| "E" car | lier document published on or after the international filing date | "X" document of par | ticular relevance; the | edaimed invention cannot be | | | | |
| cite | ument which may throw doubts on priority claim(s) or which is d to establish the publication date of another citation or other | when the docume | ent is taken alone | - | | | | |
| | mial reason (as specified) ument referring to an oral disclosure, use, exhibition or other uns | considered to invo | dve an inventive step t | claimed invention cannot be when the document is combined ents, such combination being | | | | |
| "P" door | nment published prior to the international filing date but later n the priority date claimed | | r of the same patent : | family | | | | |
| | actual completion of the international search | Date of mailing of the international search report | | | | | | |
| 29 DECE | MBER 2000 | 25 JAN2001 | | | | | | |
| | ailing address of the ISA/US er of Patents and Trademarks | Authorized officer Use Bridges ARDIN MARSOHEL | | | | | | |
| Washington | , D.C. 20231 | ARDIN MARSOHEL | | | | | | |
| Facsimile No | o. (703) 305-3230 | Telephone No. (709 | N 508-0196 | (1) | | | | |

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

| C (Continua | tion). DOCUMENTS CONSIDERED TO BE RELEVANT | | |
|-------------|--|------------|-----------------------|
| Category* | Citation of document, with indication, where appropriate, of the relevant | passages | Relevant to claim No. |
| Y | AHMAD et al. WD Repeats of the p48 Subunit of Chicken Chromatin Assembly Factor-1 Required for in Vitro Interwith Chicken Histone Deacetylase-2. The Journal of Biol Chemistry. 04 June 1999, Volume 274, Number 23, pages 16653, see especially the abstract. | 1-19 | |
| Y | JOHN et al. Rhizobium NodB protein involved in nodulasignal synthesis is a chitooligosaccharide deacetylase. Proof the National Academy of Sciences, USA. January 1993 90, pages 625-629, see especially the abstract. | ceedings | 1-19 |
| A | US 5,780,594 A (CARTER) 14 July 1998, see the entire di | isclosure. | 1-19 |
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INTERNATIONAL SEARCH REPORT

International application No. PCT/US00/24700

| A. CLASSIFICATION | OF | SUBJECT | MATTER |
|-------------------|----|---------|--------|
| US CL. | | | |

530/350 and 435/7.9

B. FIELDS SEARCHED
Minimum documentation searched
Classification System: U.S.

530/300,888,850; 435/6,7.2; 514/2

B. FIELDS SEARCHED

Electronic data bases consulted (Name of data base and where practicable terms used):

CAS, BIOTECH ABS, MEDLINE, EMBASE, WPI, WEST covering search terms: deacetylase, human, crystal, histone, inhibitor, x-ray, and crystallography

